Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	5154	((544/326,328,329,330,331,332) or (514/256,275)).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2005/01/21 17:05
L2	10068	((546/194,208,209) or (544/238, 264,336,409) or (514/252.03,255. 05,263.22,318,322,326)).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2005/01/21 17:06
L3	2091494	"2004".py. or "2005".py.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2005/01/21 17:06
L4	525	1 and 3	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR .	ON	2005/01/21 17:07
L5	10420	2 or 4	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2005/01/21 17:07

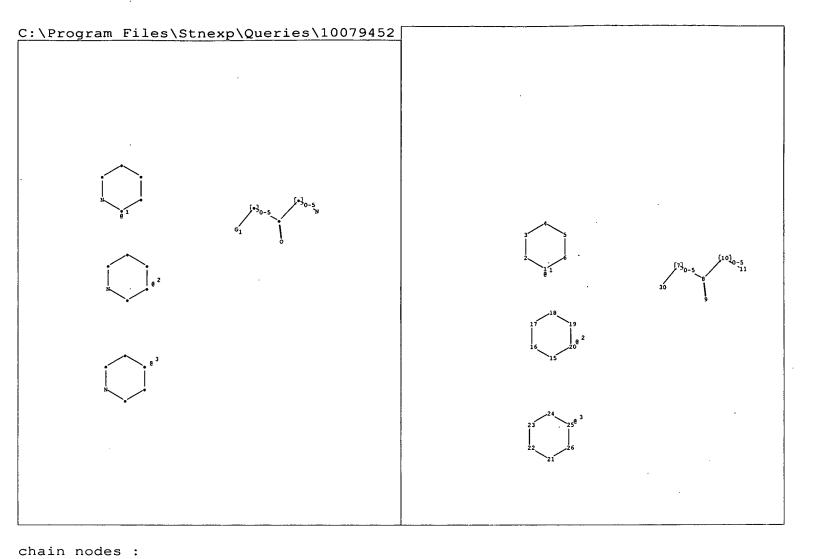
```
C:\Program Files\Stnexp\Queries\10079452
```

```
7 8 9 10
                11
                     14
                         15
                              19
                                  20
                                      21
                                          22
                                              23
                                                  27
                                                      29
                                                           30
                                                               31
                                                                   32
                                                                       35
                                                                           36
                                                                               37
    46 47 48
                116
ring nodes :
                5 6
                      16 17 18 50
                                      51
                                           52 53 54
                                                       55
                                                            56
                                                                57
                                                                   58
                                                                       59
                                                                            60
           63
                64 65 66 67 68
                                    69
                                         70
                                             71
                                                 72
                                                     73 74
                                                             75 76
                                                                      77 78
                                                                              79
    80
       81
            82
                83 84
                       85
                             86
                                 87
                                     88
                                         89
                                             90
                                                 91
                                                     92
                                                          93
                                                              94
                                                                  95
                                                                      96
                                                                          97
                                                                              98
    99
        100 101 102
                       103
chain bonds :
    2-46 7-8
              7-9 9-10 10-11 14-15 14-18 16-19 20-21
                                                               20-22
                                                                      22-23
    27-29
          27-30 30-31 31-32
                               35-36 36-37 47-48 48-116
ring bonds :
    1-2
             2-3
                   3-4
                        4-5
                             5-6
        1-6
                                  16-17
                                         16-18
                                                 17-18
                                                        50-51
                                                                50-55
                                                                       51-52
    52-53
           53-54
                  54-55
                         56-57
                                56-61
                                        57-58
                                               58-59
                                                      59-60
                                                             60-61
                                                                     62-63
                                                                            62-67
    63-64
           64-65
                  65-66
                         66-67
                                 68-69
                                        68-73
                                               69-70
                                                      70-71
                                                              71-72
                                                                     72-73
                                                                            74-75
    74-79
           75-76
                  76-77
                         77-78
                                 78-79
                                        80-81
                                               80-85
                                                      81-82
                                                              82-83
                                                                     83-84
                                                                            84 - 85
    86-87
           86-91
                  87-88
                                89-90
                         88-89
                                        90-91
                                               92-93
                                                      92-97
                                                              93 - 94
                                                                     94-95
                                                                            95-96
                  98-103
    96-97
           98-99
                         99-100
                                  100-101
                                           101-102
                                                     102-103
exact/norm bonds :
    1-2 1-6 2-3
                   2-46
                         3-4 4-5
                                   5-6
                                        7-8
                                              7-9 10-11 14-15 16-19 20-21
    22-23
          27-29
                 27-30
                         36-37
                                47-48
                                        48-116
exact bonds :
    9-10 14-18
                 16-17
                        16-18
                               17-18
                                       20-22
                                              30-31
                                                     31 - 32
                                                             35-36
normalized bonds :
    50-51
           50-55
                  51-52
                         52-53
                                 53-54
                                        54-55
                                               56-57
                                                      56-61
                                                              57-58
                                                                     58-59
                                                                            59-60
    60-61
           62-63
                  62-67
                         63-64
                                 64-65
                                        65-66
                                               66-67
                                                      .68-69
                                                                     69-70
                                                                            70-71
                                                              68-73
    71-72
           72-73
                  74 - 75
                         74-79
                                75-76
                                        76-77
                                               77-78
                                                      78-79
                                                              80-81
                                                                     80-85
                                                                            81-82
    82-83
           83-84
                  84 - 85
                         86-87
                                 86-91
                                        87-88
                                               88-89
                                                      89-90
                                                              90-91
                                                                     92-93
                                                                            92-97
    93-94
           94-95
                  95-96
                         96-97
                                 98-99
                                        98-103
                                                99-100
                                                        100-101
                                                                101-102
    102-103
isolated ring systems :
    containing 1 : 16 : 50 : 56 : 62 : 68 : 74 : 80 : 86 : 92 : 98 :
```

chain nodes :

```
G2: [*1], [*2], [*3], [*4], [*5]
G3: [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13], [*14]
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom
                                                    7:CLASS
                                                             8:CLASS
                                                                       9:CLASS
    10:CLASS
              11:Atom 14:CLASS
                                 15:CLASS
                                           16:Atom
                                                    17:Atom
                                                             18:Atom
                                                                       19:Atom
                                                    29:CLASS 30:CLASS
                        22:CLASS
                                           27:CLASS
    20:CLASS
              21:CLASS
                                  23:Atom
                                                   46:CLASS
                                                              47:CLASS
              32:Atom
                       35:CLASS
                                 36:CLASS
                                           37:Atom
    31:CLASS
    48:CLASS
              50:Atom 51:Atom 52:Atom 53:CLASS 54:Atom 55:CLASS 56:Atom
    57: Atom 58: Atom 59: Atom 60: Atom 61: Atom 62: Atom 63: Atom 64: CLASS
    65:CLASS
             66:CLASS
                        67:Atom 68:Atom 69:Atom 70:Atom 71:Atom
                                                                     72:Atom
                      75:Atom
                              76:Atom
                                        77:Atom
                                                 78:Atom
                                                          79:Atom
    73:Atom
             74:Atom
                                                                   80:Atom
    81:Atom
             82:Atom
                      83:Atom
                               84:Atom
                                        85:Atom
                                                 86:Atom
                                                          87:Atom
    89:Atom
             90:Atom
                      91:Atom
                               92:Atom 93:Atom
                                                 94:Atom
                                                          95:Atom
                                                                   96:Atom
    97:Atom
             98:Atom
                      99:Atom 100:Atom 101:Atom 102:Atom
                                                             103:Atom
    114:CLASS 116:CLASS
Generic attributes :
    11:
    Saturation
                          : Unsaturated
    19:
    Saturation
                           : Unsaturated
    23:
    Saturation
                           : Unsaturated
    32:
    Saturation
                           : Unsaturated
    37:
    Saturation
                           : Unsaturated
Element Count :
```

Node 47: Limited C,C1-5



```
7 8 9 10 11 30

ring nodes:

1 2 3 4 5 6 15 16 17 18 19 20 21 22 23 24 25 26

chain bonds:

7-8 7-30 8-9 8-10 10-11

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20

21-22 21-26 22-23 23-24 24-25 25-26

exact/norm bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-30 8-9 10-11 15-16 15-20 16-17 17-18

18-19 19-20 21-22 21-26 22-23 23-24 24-25 25-26

exact bonds:

7-8 8-10
```

G1:[*1],[*2],[*3]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 30:CLASS

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

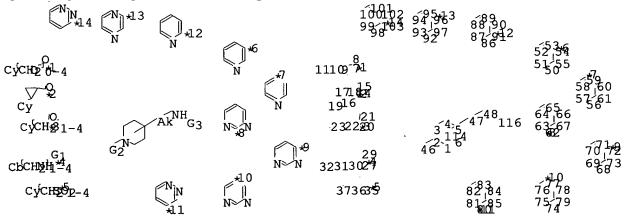
=> screen 1840

L1 SCREEN CREATED

=> screen 2016 OR 2039 OR 2040 OR 2045 OR 2047

L2 SCREEN CREATED

=> Uploading C:\Program Files\Stnexp\Queries\10079452 (rce7).str



chain nodes : 7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 48 116 ring nodes : 5 6 16 17 18 50 51 52 53 54 55 56 57 58 59 60 61 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 63 64 65 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103

```
chain bonds :
2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30
 30-31 31-32 35-36 36-37 47-48 48-116
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 50-51 50-55 51-52 52-53
53-54 54-55 56-57 56-61 57-58 58-59 59-60 60-61 62-63 62-67 63-64 64-65 65-66 66-67 68-69 68-73 69-70 70-71 71-72 72-73 74-75 74-79 75-76 76-77 77-78 78-79 80-81 80-85 81-82 82-83 83-84 84-85 86-87 86-91 87-88 88-89
89-90 90-91 92-93 92-97 93-94 94-95 95-96 96-97
                                                           98-99 98-103 99-100
100-101 101-102 102-103
exact/norm bonds :
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 10-11 14-15 16-19 20-21 22-23
27-29 27-30 36-37 47-48 48-116
exact bonds :
9-10 14-18 16-17 16-18 17-18 20-22 30-31 31-32 35-36
normalized bonds :
50-51 50-55 51-52 52-53 53-54 54-55 56-57 56-61 57-58 58-59 59-60 60-61
62-63 62-67 63-64 64-65 65-66 66-67 68-69 68-73 69-70 70-71 71-72 72-73
74-75 74-79 75-76 76-77 77-78 78-79 80-81 80-85 81-82 82-83 83-84 84-85
86-87 86-91 87-88 88-89 89-90 90-91 92-93 92-97 93-94 94-95 95-96 96-97
98-99 98-103 99-100 100-101 101-102 102-103
isolated ring systems :
containing 1: 16: 50: 56: 62: 68: 74: 80: 86: 92: 98:
G1:0,N
G2: [*1], [*2], [*3], [*4], [*5]
G3: [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13], [*14]
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom 35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:Atom 51:Atom
52:Atom 53:CLASS 54:Atom 55:CLASS 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 63:Atom 64:CLASS 65:CLASS 66:CLASS 67:Atom 68:Atom 69:Atom
70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom
79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 85:Atom 86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:Atom 93:Atom 94:Atom 95:Atom
97:Atom 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom 103:Atom 114:CLASS
116:CLASS
Generic attributes :
11:
              : Unsaturated
Saturation
19:
Saturation
                       : Unsaturated
23:
               : Unsaturated
Saturation
32:
Saturation
              : Unsaturated
37:
Saturation
              : Unsaturated
```

Element Count:
Node 47: Limited
C,C1-5

L3 STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4 QUE L3 AND L1 NOT L2

=> d 14

L4 HAS NO ANSWERS

L1 SCR 1840

L2 SCR 2016 OR 2039 OR 2040 OR 2045 OR 2047

L3 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation. L4 $\,$ QUE L3 AND L1 NOT L2 $\,$

=> s 14 sss sam

SAMPLE SEARCH INITIATED 13:50:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3223 TO ITERATE

31.0% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

5 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 61056 TO 67864
PROJECTED ANSWERS: 82 TO 562

L5 5 SEA SSS SAM L3 AND L1 NOT L2

=> => s 14 sss ful

FULL SEARCH INITIATED 13:51:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62610 TO ITERATE

100.0% PROCESSED 62610 ITERATIONS SEARCH TIME: 00.00.02

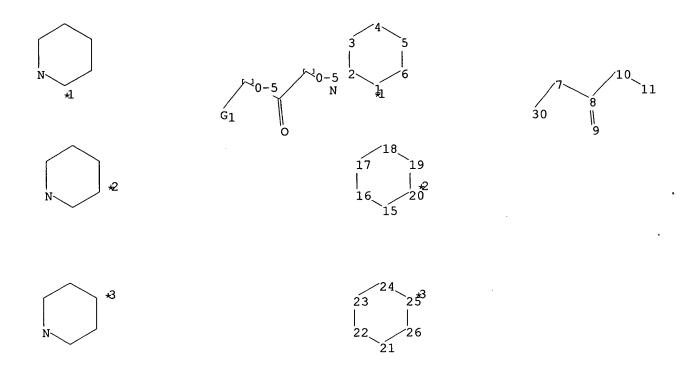
231 ANSWERS

SEARCH TIME: 00.00.02

L6 231 SEA SSS FUL L3 AND L1 NOT L2

=>

Uploading C:\Program Files\Stnexp\Queries\10079452 (rce sub).str



chain nodes :
7 8 9 10 11 30
ring nodes :
1 2 3 4 5 6 15 16 17 18 19 20 21 22 23 24 25 26
chain bonds :
7-8 7-30 8-9 8-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20 21-22
21-26 22-23 23-24 24-25 25-26
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-30 8-9 10-11 15-16 15-20 16-17 17-18 18-19
19-20 21-22 21-26 22-23 23-24 24-25 25-26
exact bonds :
7-8 8-10

G1:[*1],[*2],[*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 30:CLASS

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7

STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 17 sub=16 sss sam

SAMPLE SUBSET SEARCH INITIATED 13:55:04 FILE 'REGISTRY' SAMPLE SUBSET SCREEN SEARCH COMPLETED - 16 TO ITERATE

100.0% PROCESSED 16 ITERATIONS 4 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):

ONLINE **COMPLETE**

80 TO 560

PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):

4 TO 200

4 SEA SUB=L6 SSS SAM L7 L8

=> => s 17 sub=16 sss ful

FULL SUBSET SEARCH INITIATED 13:55:49 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED - 230 TO ITERATE

100.0% PROCESSED 230 ITERATIONS

24 ANSWERS

SEARCH TIME: 00.00.01

L9

24 SEA SUB=L6 SSS FUL L7

=> s 16 not 19

L10 207 L6 NOT L9

=> => s 110

L11 7 L10

=> d 111 1-7 bib, ab, hitstr

```
ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
L11
     2004:1080888 CAPLUS
AN
DN
     142:56340
TΙ
     4-Heteroarylamino-substituted 3-fluoro-piperidines as NMDA/NR2B
     antagonists, and their preparation, pharmaceutical compositions, and
     methods of use
     Liverton, Nigel J.; Claiborne, Christopher F.; Claremon, David A.;
IN
     McCauley, John A.
PA
    Merck & Co., Inc., USA
     PCT Int. Appl., 41 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                            APPLICATION NO.
                                                                   DATE
                                            _____
                                                                   _____
    WO 2004108705
PΙ
                         A1
                                20041216
                                            WO 2004-US17175
                                                                   20040528
        W: AE, AG, AL, AM, AT, AU, AZ,
                                         🔏A, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, QE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
PRAI US 2003-475938P
                                20030604
     Title compds. I and their pharmaceutically acceptable salts are disclosed
     [wherein: HetAr is a 5- or 6-membered heteroarom. ring containing 1 or 2 N
     ring atoms, thiazolyl, or thiadiazolyl; HetAr is optionally substituted
     with 1 or 2 substituents, each substituent independently is C1-4 alkyl, F,
     Cl, Br, or iodo; A is a bond or C1-2 alkylene; and B is
     aryl-(CH2)0-3OC(0)-, indanyl-(CH2)0-3OC(0)-, aryl-(CH2)1-3C(0)-,
     arylcyclopropyl-C(O)-, or aryl-(CH2)1-3NHC(O)-, wherein any aryl is
     optionally substituted by 1-5 substituents, each substituent is
     independently C1-4 alkyl, F, or Cl]. I are effective as NMDA NR2B
     antagonists, useful for treating conditions such as, for example,
     Parkinson's disease, Alzheimer's disease, migraine, epilepsy and pain.
     Seven specific examples are claimed, and these plus various salts were
     prepared For instance, invention compound II was prepared in 8 steps: (1)
     coupling of CDI with 4-MeC6H4CH2OH and 4-piperidone HCl; (2)
     \alpha-fluorination of the piperidone carbonyl; (3) Witting reaction of
     the piperidone carbonyl with Ph3P:CHCO2Et; (4) stereoselective reduction of
     the resulting olefin to give primarily cis-isomeric ester III; (5) alkaline
     saponification of the Et ester; (6) conversion of the resulting acid to an
amine
     with diphenylphosphoryl azide; (7) heteroarylation of the amine with
     2-chloropyrimidine; and (8) chiral HPLC. In both (1) a cell-based
     functional assay to determine IC50 for inhibition of NR1A/NR2B receptors in
     Ltk- cells, and (2) a radioligand binding assay using tritiated AMD-2
     (preparation given) to determine Ki, compds. I had values of less than 50 μM,
     with these values advantageously being even lower than 0.1 \mu M.
     808732-98-1P, (-)-(3S,4R)-4-Methylbenzyl 3-fluoro-4-[(pyrimidin-2-
IT
     ylamino)methyl]piperidine-1-carboxylate
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
```

Absolute stereochemistry. Rotation (-).

IT 808732-99-2P, (+)-(3R,4S)-4-Methylbenzyl 3-fluoro-4-[(pyrimidin-2ylamino)methyl]piperidine-1-carboxylate 808733-00-8P, (-)-trans-4-Methylbenzyl 3-fluoro-4-[(pyrimidin-2ylamino)methyl]piperidine-1-carboxylate 808733-01-9P, (+)-trans-4-Methylbenzyl 3-fluoro-4-[(pyrimidin-2ylamino)methyl]piperidine-1-carboxylate 808733-02-0P, (-)-N-[(3S,4R)-cis-3-Fluoro-1-[((1R,2R)-2-phenylcyclopropyl)carbonyl]piperidin-4-yl]methyl]pyrimidin-2-amine 808733-05-3P, cis-4-Methylbenzyl 3-fluoro-4-[(pyrimidin-2-ylamino)methyl]piperidine-1carboxylate 808733-06-4P, (-)-(3S,4R)-4-Methylbenzyl3-fluoro-4-[(pyrimidin-2-ylamino)methyl]piperidine-1-carboxylate hydrochloride 808733-07-5P, (+)-(3R,4S)-4-Methylbenzyl3-fluoro-4-[(pyrimidin-2-ylamino)methyl]piperidine-1-carboxylate hydrochloride 808733-08-6P, (-)-trans-4-Methylbenzyl 3-fluoro-4-[(pyrimidin-2-ylamino)methyl]piperidine-1-carboxylate hydrochloride 808733-09-7P, (+)-trans-4-Methylbenzyl 3-fluoro-4-[(pyrimidin-2-ylamino)methyl]piperidine-1-carboxylate hydrochloride 808733-10-0P, (-)-N-[[(3S,4R)-cis-3-Fluoro-1-[((1R,2R)-2-phenylcyclopropyl)carbonyl]piperidin-4-yl]methyl]pyrimidin-2amine hydrochloride RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of heteroarylamino-substituted fluoropiperidines as NMDA/NR2B receptor antagonists) RN808732-99-2 CAPLUS CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, (3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 808733-00-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, (3R,4R)-rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

RN 808733-01-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, (3R,4R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

RN 808733-02-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Rotation (-).

RN 808733-05-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 808733-06-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, monohydrochloride, (3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

RN 808733-07-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, monohydrochloride, (3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

HCl

RN 808733-08-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, monohydrochloride, (3R,4R)-rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

HCl

RN 808733-09-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-fluoro-4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester, monohydrochloride, (3R,4R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

HCl

RN 808733-10-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Rotation (-).

● HCl

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
L11
AN
     2004:412925 CAPLUS
DN
     141:7135
ΤI
     Preparation of N-(arylacetyl) cyclic amine derivatives as orexin
     antagonists
     Chan, Wai Ngor; Nash, David John; Porter, Roderick Alan; Stead, Rachel
IN
     Elizabeth Anne
PA
     Glaxo Group Limited, UK
SO
     PCT Int. Appl., 25 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                            APPLICATION NO.
                                                                   DATE
                                            _____
                                                                   _____
                                20040521
                                            WO 2003-EP12407
                                                                   20031104
PI
    WO 2004041791
                          Α1
        W: AE, AG, AL, AM, AT, AU, AZ
                                        BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI GB 2002-25944
                          Α
                                20021106
    MARPAT 141:7135
     The title compds. [I; Y = a bond, O, NQ, (CH2)n (wherein n = 1-3); m = 1-3
AΒ
     0-1; X = NR (R = H, alkyl); Q = H, alkyl; Arl = (un)substituted aryl, mono
     or bicyclic heteroaryl group containing up to 4 heteroatoms selected from N, O
     and S; Ar2 = (un)substituted Ph, 5-6 membered heterocyclyl group containing up
     to 4 heteroatoms selected from N, O and S, or substituted bicyclic aromatic
     or bicyclic heteroarom. group containing up to 4 heteroatoms selected from N,
     O and S; R1, R2 = H, (un) substituted amino, alkyl or Ph] which are
     non-peptide antagonists of human orexin receptors, in particular orexin-1
     receptors, were prepared Thus, reacting 2-methoxyphenylacetic acid with
     (S)-2-[(6,7-difluoroquinoxalin-2-ylamino)methyl]piperidine afforded 70%
     1-{(S)-2-[(6,7-difluoroquinoxalin-2-ylamino)methyl]piperidin-1-yl}-2-(2-
     methoxyphenyl)ethanone. The exemplified compds. I showed pKb values in
     the range 6.8 to 8.9 at the human cloned orexin-1 receptor, and pKb values
     in the range < 6.7 to 8.2 at the human cloned orexin-2 receptor. In
     particular, the compds. I are of potential use in the treatment of
     obesity, including obesity observed in Type 2 (non-insulin-dependent)
     diabetes patients, and/or sleep disorders. Addnl. the compds. I are
     useful in the treatment of stroke, particularly ischemic or hemorrhagic
     stroke, and/or blocking the emetic response, i.e. useful in the treatment
     of nausea and vomiting. The pharmaceutical composition comprising the
compound I
     is claimed.
IT
     691372-59-5P 691372-60-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of N-(arylacetyl) cyclic amines as orexin antagonists)
RN
     691372-59-5 CAPLUS
     2-Piperidinemethanamine, N-(5-bromo-2-pyrimidinyl)-1-[(2-
     methoxyphenyl)acetyl]-, (2S)- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

RN 691372-60-8 CAPLUS

CN 2-Piperidinemethanamine, N-(5-bromo-2-pyrimidinyl)-1-[(2-ethoxyphenyl)acetyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

```
ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
L11
     2002:964146 CAPLUS
AN
DN
     138:39187
ΤI
     Preparation of piperidinecarboxylates and related compounds as NMDA NR2B
     receptor antagonists for the treatment or prevention of migraine.
     Allen, Christopher; Koblan, Ken S.; Sleeth, Timothy
IN
PA
     Merck & Co., Inc., USA
                                 Comprow Arsigner
SO
     PCT Int. Appl., 185 pp.
     CODEN: PIXXD2
DΨ
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                        KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
     _____
                         ____
                                            ______
                                                                   _____
     WO 2002100352
                         A2
                                20021219
                                            WO 2002-US21069
                                                                   20020607
PΙ
                                20030327
     WO 2002100352
                         A3
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
            LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
            UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
             GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
             GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1399160
                         A2
                                20040324
                                            EP 2002-744807
                                                                   20020607
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                                                                   20031205 - 7 no DP.
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004537526
                                20041216
                                            JP 2003-503178
                          Т2
                                            US 2003-479923
     US 2004204341
                          A1
                                20041014
                                20010612
PRAI US 2001-297672P
                          P
     WO 2002-US21069
                         W
                                20020607
AB
     A method for treating or preventing migraines comprises administration of
     an NR2B receptor antagonist (no data). The invention also encompasses the
     combination of an NR2B antagonist with a cyclooxygenase-2 selective
     inhibitor, a calcitonin gene-related peptide receptor (CGRP) ligand, a
     leukotriene receptor antagonist, or a 5HT1B/1D agonist for the treatment
     or prevention of migraines. Thus, 4-hydroxybenzoic acid,
     1-hydroxybenzotriazole hydrate, benzyl 4-(aminomethyl)piperidine-1-
     carboxylate (preparation given), and Et3N in DMF were treated with
     1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride and the mixture
     allowed to stir at room temperature for 18 h to give 4-[(4-
     hydroxybenzoylamino)methyl]piperidine-1-carboxylic acid benzyl ester.
IT
     455265-37-9P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of piperidinecarboxylates and related compds. as NR2B receptor
        antagonists for the treatment or prevention of migraine)
     455265-37-9 CAPLUS
RN
     1-Piperidinecarboxylic acid, 4-[[[2-(methylthio)-4-
CN
     pyrimidinyl]amino]methyl]-, (4-methylphenyl)methyl ester (9CI)
                                                                     (CA INDEX
```

NAME)

MeS

ester (9CI)

(CA INDEX NAME)

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NH-CH<sub>2</sub>
IT
     455265-19-7P, Benzyl 4-[(4-pyridinylamino)methyl]-1-
    piperidinecarboxylate 455265-20-0P, Benzyl 4-[[(3-
    pyridinyl)amino]methyl]-1-piperidinecarboxylate 455265-24-4P
     455265-25-5P, 4-[(3-Methylpyridin-4-ylamino)methyl]piperidine-1-
     carboxylic acid benzyl ester 455265-27-7P, Benzyl
     4-[[(4-methyl-2-pyridinyl)amino]methyl]-1-piperidinecarboxylate
     455265-30-2P 455265-31-3P 455265-32-4P, Benzyl
     4-[[(2-pyridinyl)amino]methyl]-1-piperidinecarboxylate
     455265-33-5P, Benzyl 4-[[(4-ethyl-2-pyridinyl)amino]methyl]-1-
    piperidinecarboxylate 455265-34-6P, Benzyl 4-[[(1-oxido-4-
    pyridinyl)amino]methyl]-1-piperidinecarboxylate 455265-35-7P
     455265-36-8P 455265-38-0P 455265-39-1P
     455265-40-4P 455265-41-5P 455265-42~6P
     455265-44-8P 455265-45-9P 455265-48-2P
     455265-49-3P 455265-51-7P 455265-52-8P
     455265-54-0P 455265-55-1P 455265-56-2P
     455265-57-3P 455265-58-4P 455265-59-5P
     455265-60-8P 455265-61-9P 455265-62-0P
     455265-63-1P 455265-64-2P 455265-66-4P
     455265-67-5P 455265-68-6P 455265-69-7P
     455265-70-0P 455265-71-1P 455265-73-3P
     455265-74-4P 455265-75-5P 455265-76-6P
     455265-77-7P 455265-78-8P 455265-79-9P
     455265-80-2P 455265-81-3P 455265-82-4P
     455265-83-5P 455265-84-6P 455265-85-7P
     455265-86-8P 455265-88-0P 455265-89-1P
     455265-90-4P 455265-91-5P 455265-94-8P
     455265-95-9P 455265-98-2P 455265-99-3P
     455266-00-9P 455266-01-0P 455266-03-2P
     455266-04-3P 455266-05-4P 455266-06-5P
     455266-07-6P 455266-08-7P 455266-11-2P
     455266-12-3P 455266-14-5P 455266-15-6P
     455266-22-5P 455266-25-8P 455266-26-9P
     455266-28-1P 455266-29-2P 455266-98-5P
     455267-18-2P 455267-73-9P 455267-78-4P
     455267-93-3P 455267-94-4P 455267-96-6P
     455268-07-2P 455290-06-9P, Benzyl 4-[[(5-methyl-2-
    pyridinyl)amino]methyl]-1-piperidinecarboxylate 455290-15-0P
     478552-71-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of piperidinecarboxylates and related compds. as NR2B receptor
        antagonists for the treatment or prevention of migraine)
RN
     455265-19-7 CAPLUS
CN
     1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, phenylmethyl
```

RN 455265-20-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(3-pyridinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$O$$

$$CH_2-NH$$

$$N$$

RN 455265-24-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

RN 455265-25-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methyl-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$0$$

$$Me$$

$$Me$$

RN 455265-27-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(4-methyl-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} \\ & & \\ & & \\ \end{array}$$

RN 455265-30-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\$$

RN 455265-31-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-32-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyridinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{CH}_2-\text{NH} & & \\ & & \\ \text{N} & & \\ \end{array}$$

RN 455265-33-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(4-ethyl-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-34-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(1-oxido-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

RN 455265-35-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyrimidinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} \\ & & \\ & & \\ \end{array}$$

RN 455265-36-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-2-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$0$$

$$N$$

$$Me$$

RN 455265-38-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-chloro-3-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$CH_2-NH$$

$$CH_2-NH$$

$$CH_2-NH$$

$$CH_2-NH$$

RN 455265-39-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(pyrazinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-40-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methyl-2-pyridinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & \\ \hline \\ NH-CH_2 \\ \hline \end{array}$$

RN 455265-41-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (2-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-42-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (2-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-44-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-chloro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & Cl \\ \hline Ph-CH_2-O-C & & & & N & N \\ \hline \end{array}$$

RN 455265-45-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(3-pyridazinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-48-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (3-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-49-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-51-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(1,6-dihydro-6-oxo-3-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-52-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methyl-2-pyridinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-54-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 455265-55-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (4-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-56-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

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RN 455265-57-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(4-pyridinylamino)methyl]-, (4-methylphenyl)methyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-58-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-cyano-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-59-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloropyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ & & & & & \\ \text{Ph-CH}_2-\text{O-C} & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ \end{array}$$

RN 455265-60-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-(hydroxymethyl)-4-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ N & & & \\ \hline N & & & \\ CH_2-OH & & & \\ \end{array}$$

RN 455265-61-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(4-pyridinylamino)methyl]-, phenylmethyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-62-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(2-pyridinylamino)methyl]-, phenylmethyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-63-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[3-(trifluoromethyl)-2-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-64-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[(methylamino)methyl]-4-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH-CH}_2 \\ & \text{N} \\ & \text{CH}_2 - \text{NHMe} \\ & \text{O} \\ \end{array}$$

RN 455265-66-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & \\ & & \\ &$$

RN 455265-67-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(4-pyridinylamino)methyl]-, (4-ethylphenyl)methyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-68-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloro-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 \\ CH_2-NH \\ \hline \\ N \\ \end{array}$$

RN 455265-69-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3,4-dihydro-3-oxopyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-70-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[(dimethylamino)methyl]-4-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} \\ & & \\ & & \\ \end{array}$$

RN 455265-71-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-chloro-4-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-73-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-chloro-6-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-74-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 455265-75-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \\ \text{N} \\ \text{N} \end{array}$$

$$\text{NH-CH}_2$$

RN 455265-76-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridazinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-77-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-chloro-4-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$C1$$

$$N$$

RN 455265-78-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-bromo-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-79-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-80-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
Me \\
N - C - O - CH_2
\end{array}$$
Me

RN 455265-81-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-amino-6-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$NH_2$$
 NH_2
 $C-O-CH_2-Ph$
 NH_2
 NH_2

RN 455265-82-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridazinylamino)methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-83-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-chloro-5-fluoro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-84-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$Ph-CH_2-NH$$

$$F$$

RN 455265-85-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-cyclopropylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-86-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ \text{Ph-CH}_2-\text{CH}_2-\text{S} \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-88-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-hydroxy-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-89-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-90-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-91-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[1-(4-pyridinylamino)ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-94-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-95-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-98-2 CAPLUS

CN 4-Piperidinemethanamine, N-(4-methyl-2-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455265-99-3 CAPLUS

CN 4-Piperidinemethanamine, N-(3-methylpyrazinyl)-1-[(2-phenylethyl)sulfonyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 455266-00-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-methylphenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

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RN 455266-01-0 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-fluorophenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & \parallel \\
 & N \\
 & N \\
 & N \\
 & N \\
 & O \\$$

RN 455266-03-2 CAPLUS

CN 4-Pyrimidinecarboxamide, 2-[[[1-[(2-phenylethyl)sulfonyl]-4-piperidinyl]methyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \parallel & C \\ \parallel & C$$

RN 455266-04-3 CAPLUS

CN 4-Piperidinemethanamine, N-(3-chloropyrazinyl)-1-[(2-phenylethyl)sulfonyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & \\ & & & & & & \\ & & & & & \\ \text{Ph-CH}_2-\text{CH}_2-\text{S} & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ \end{array}$$

RN 455266-05-4 CAPLUS

CN 4-Piperidinemethanamine, N-(5-methyl-4-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2\text{-CH}_2\text{-S} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-06-5 CAPLUS

CN 4-Piperidinemethanamine, N-(4-amino-5-fluoro-2-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
F & O \\
N & S - CH_2 - CH_2 - Ph \\
N & O \\
N$$

RN 455266-07-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2-fluorophenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ N & & \\ NH-CH_2 & & \\ & & \\ O & & \\ \end{array}$$

RN 455266-08-7 CAPLUS

CN 4-Piperidinemethanamine, N-(6-amino-5-nitro-2-pyridinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & & \\ \text{NH}_2 & & & & & & & & \\ \text{O}_2\text{N} & & & & & & & \\ \text{N} & & & & & & & \\ \text{N} & & & & & & & \\ \text{NH}_2 & & & & & & \\ \text{N} & & & & & & \\ \text{NH}_2 & & & & & \\ \text{N} & & & & & \\ \text{NH}_2 & & & & & \\ \text{NH}_2 & & & & & \\ \text{NH}_2 & & &$$

RN 455266-11-2 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-pyrazinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2\text{-CH}_2\text{-} & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-12-3 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-4-pyrimidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ \text{Ph-CH}_2-\text{CH}_2-\text{S} \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-14-5 CAPLUS

CN 4-Piperidinemethanamine, N-(4-amino-2-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455266-15-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-chlorophenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

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RN 455266-22-5 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylcyclopropyl)carbonyl]-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ C & N \end{array}$$

RN 455266-25-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[1-oxo-4-(2-thienyl)butyl]-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

$$S$$
 CH_2 3 C N CH_2 N N

RN 455266-26-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, 3-thienylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 455266-28-1 CAPLUS
CN 4-Piperidinemethanamine, 1-(1-oxo-3-phenylpropyl)-N-2-pyrimidinyl- (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2\text{-CH}_2\text{-C} & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-29-2 CAPLUS

CN 1-Piperidinecarboximidamide, N-cyano-N'-(phenylmethyl)-4-[(4-pyridinylamino)methyl]- (9CI) (CA INDEX NAME)

$$Ph-CH_2-N=C$$

$$NC-NH$$

RN 455266-98-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloropyrazinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & & \\ N & \\ NH-CH_2 & & \\ \end{array}$$

RN 455267-18-2 CAPLUS

CN 4-Piperidinemethanamine, N-(2-chloro-5-methyl-4-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455267-73-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-chloro-5-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455267-78-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5,6-dichloro-4-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
N & NH - CH_2 \\
N & C1 \\
C1 & C - O - CH_2 - Ph_1
\end{array}$$

RN 455267-93-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-chloro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

HCl

RN 455267-94-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-hydroxy-4-[(4-pyridinylamino)methyl]-, phenylmethyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 455265-72-2 CMF C19 H23 N3 O3

Ph-CH₂-O-C
$$N$$
 N
 N

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455267-96-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-fluoro-4-pyridinyl)amino]methyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455267-68-2 CMF C19 H22 F N3 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455268-07-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (3-fluorophenyl)methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455265-53-9 CMF C19 H22 F N3 O2

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455290-06-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455290-15-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

Me
$$NH-CH_2$$
 $N-C-O-CH_2$ $N-C-O-CH_2$

RN 478552-71-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methyl-2-pyridinyl)amino]methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & & & \\ & \parallel & \\ NH-CH_2 & & & \\ & N & & \end{array}$$

IT 455267-76-2

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of piperidinecarboxylates and related compds. as NR2B receptor antagonists for the treatment or prevention of migraine)

RN 455267-76-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[5-chloro-2,6-bis(methylthio)-4-pyrimidinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

IT 455267-07-9P, (cis)-3-Hydroxy-4-[(2,3,5,6-tetrachloropyridin-4-ylamino)methyl]piperidine-1-carboxylic acid benzyl ester

455267-08-0P 455267-15-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of piperidinecarboxylates and related compds. as NR2B receptor antagonists for the treatment or prevention of migraine)

RN 455267-07-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[[(2,3,5,6-tetrachloro-4-pyridinyl)amino]methyl]-, phenylmethyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455267-08-0 CAPLUS

CN 2-Pyridinecarboxylic acid, 4-[[[1-[(phenylmethoxy)carbonyl]-4-piperidinyl]methyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ & & & & & \\ \text{Ph-CH}_2-\text{O-C} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ \end{array}$$

RN 455267-15-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[[(2,4-dimethoxyphenyl)methyl]amino]-6-methyl-4-pyrimidinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

```
ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
L11
     2002:676010 CAPLUS
ΑN
DN
     137:216875
     Preparation of N-acyl-4-(heterocyclylaminomethyl)piperidines as NMDA/NR2B
ΤI
     antagonists
     Claiborne, Christopher F.; Butcher, John W.; Claremon, David A.; Libby,
IN
     Brian E.; Liverton, Nigel J.; Munson, Peter M.; Nguyen, Kevin T.;
     Phillips, Brian; Thompson, Wayne; McCauley, John A.
     Merck & Co., Inc., USA
PΑ
                                                                     Appl. Pci.
     PCT Int. Appl., 208 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
                         ____
                                _____
                                            _____
PΙ
     WO 2002068409
                          A1
                                20020906
                                            WO 2002-US5226
                                                                    20020220
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                          CA 2002-2438895
     CA 2438895
                          AA
                                20020906
                                                                    20020220
                                             US 2002-79452
                                                                    20020220
     US 2002165241
                          A1
                                20021107
                                             EE 2003-403
                                                                    20020220
     EE 200300403
                                20031215
                          Α
                                             EP 2002-721105
     EP 1379520
                          A1
                                20040114
                                                                    20020220
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002007526
                          Α
                                20040309
                                             BR 2002-7526
                                                                    20020220
                                20040812
                                             JP 2002-567923
                                                                    20020220
     JP 2004524314
                          Т2
     US 2004209889
                          A1
                                20041021
                                             US 2003-470561
                                                                    20030729
     NO 2003003732
                          Α
                                20031022
                                            NO 2003-3732
                                                                    20030822
PRAI US 2001-271100P
                          Ρ.
                                20010223
                                20020220
                          W
     WO 2002-US5226
OS
     MARPAT 137:216875
     BQ1(X)ANHQ2 [Q1 = 5-7 membered N-containing nonarom. ring, azabicyclooctyl; Q2
AB
     = 5-6 membered (substituted) heteroaryl ring; A = alkylene; B =
     Ar(CH2)0-302C, Ar(CH2)0-3S02, etc.; Ar = (substituted) aryl, heteroaryl; X
     = H, OH, F, alkyl, alkoxy, NH2, O], were prepared Thus,
     1-[(benzyloxy)carbonyl]-4-piperidinecarboxylic acid, 4-aminopyridine, EDC,
     and HOAt were kept 4 h in DMF to give the amide, which was reduced with
     BH3. THF to give benzyl 4-[(4-pyridylamino)methyl]-1-piperidinecarboxylate.
     Title compds. showed IC50's of <50 \mu M for inhibition of NR1A/2B NMDA
     receptor activation.
IT
     455265-19-7P 455265-20-0P 455265-24-4P
     455265-25-5P 455265-27-7P 455265-30-2P
     455265-31-3P 455265-32-4P 455265-33-5P
     455265-34-6P 455265-35-7P 455265-36-8P
     455265-37-9P 455265-38-0P 455265-39-1P
     455265-40-4P 455265-41-5P 455265-42-6P
     455265-44-8P 455265-45-9P 455265-47-1P
     455265-48-2P 455265-49-3P 455265-51-7P
     455265-52-8P 455265-53-9P 455265-54-0P
     455265-55-1P 455265-56-2P 455265-57-3P
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455265-58-4P 455265-59-5P 455265-60-8P
     455265-61-9P 455265-62-0P 455265-63-1P
     455265-64-2P 455265-66-4P 455265-67-5P
     455265-68-6P 455265-69-7P 455265-70-0P
     455265-71-1P 455265-72-2P 455265-73-3P
     455265-74-4P 455265-75-5P 455265-76-6P
     455265-77-7P 455265-78-8P 455265-79-9P
     455265-80-2P 455265-81-3P 455265-82-4P
     455265-83-5P 455265-84-6P 455265-85-7P
     455265-86-8P 455265-88-0P 455265-89-1P
     455265-90-4P 455265-91-5P 455265-94-8P
     455265-95-9P 455265-98-2P 455265-99-3P
     455266-00-9P 455266-01-0P 455266-03-2P
     455266-04-3P 455266-05-4P 455266-06-5P
     455266-07-6P 455266-08-7P 455266-11-2P
     455266-12-3P 455266-14-5P 455266-15-6P
     455266-22-5P 455266-25-8P 455266-26-9P
     455266-28-1P 455266-29-2P 455266-30-5P
     455266-31-6P 455266-32-7P 455266-33-8P
     455266-34-9P 455266-35-0P 455266-36-1P
     455266-37-2P 455266-40-7P 455266-41-8P
     455266-42-9P 455266-43-0P 455266-44-1P
     455266-45-2P 455266-46-3P 455266-47-4P
     455266-48-5P 455266-50-9P 455266-51-0P
     455266-52-1P 455266-53-2P 455266-54-3P
     455266-55-4P 455266-56-5P 455266-57-6P
     455266-58-7P 455266-60-1P 455266-61-2P
     455266-62-3P 455266-63-4P 455266-64-5P
     455266-65-6P 455266-67-8P 455266-68-9P
     455266-69-0P 455266-70-3P 455266-71-4P
     455266-72-5P 455266-73-6P 455266-74-7P
     455266-75-8P 455266-76-9P 455266-78-1P
     455266-79-2P 455266-80-5P 455266-81-6P
     455266-82-7P 455266-83-8P 455266-84-9P
     455266-85-0P 455266-86-1P 455266-87-2P
     455266-88-3P 455266-89-4P 455266-91-8P
     455266-92-9P 455266-93-0P 455266-94-1P
     455266-95-2P 455266-96-3P 455266-97-4P
     455266-98-5P 455266-99-6P 455267-00-2P
     455267-02-4P 455267-03-5P 455268-07-2P
     455290-06-9P 455290-08-1P 455290-10-5P
     455290-13-8P 455305-07-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (claimed compound; preparation of
N-acyl-4-(heterocyclylaminomethyl)piperidine
        s as NMDA/NR2B antagonists)
     455265-19-7 CAPLUS
     1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, phenylmethyl
     ester (9CI)
                 (CA INDEX NAME)
```

RN

CN

RN 455265-20-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(3-pyridinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$O$$

RN 455265-24-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-25-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methyl-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-27-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(4-methyl-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} \\ & & \\ & & \\ \end{array}$$

RN 455265-30-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-31-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-32-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyridinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-33-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(4-ethyl-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-34-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(1-oxido-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 455265-35-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyrimidinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$N$$

$$N$$

$$N$$

RN 455265-36-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-2-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & \\ & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & &$$

RN 455265-37-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-(methylthio)-4-pyrimidinyl]amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 455265-38-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-chloro-3-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-39-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(pyrazinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$0$$

$$N$$

$$N$$

RN 455265-40-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methyl-2-pyridinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-41-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (2-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-42-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (2-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 455265-44-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-chloro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-45-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(3-pyridazinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-47-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloro-2-pyridinyl)amino]methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-48-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (3-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-49-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-51-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(1,6-dihydro-6-oxo-3-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} \\ & & \\ & & \\ & & \\ \end{array}$$

RN 455265-52-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methyl-2-pyridinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-53-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (3-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \\ & \parallel & \\ & \text{NH-CH}_2 & \\ & & \end{array}$$

RN 455265-54-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-55-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (4-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ N & & & \\ & & & \\ N & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 455265-56-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-57-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(4-pyridinylamino)methyl]-, (4-methylphenyl)methyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-58-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-cyano-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-59-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloropyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & \\ & & & & & & \\ Ph-CH_2-O-C & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ \end{array}$$

RN 455265-60-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-(hydroxymethyl)-4-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-61-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(4-pyridinylamino)methyl]-, phenylmethyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-62-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(2-pyridinylamino)methyl]-, phenylmethyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-63-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[3-(trifluoromethyl)-2-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-64-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[(methylamino)methyl]-4-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

NH-
$$CH_2$$
N

 $C-O-CH_2-Ph$
 CH_2-NHMe

RN 455265-66-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-pyrimidinylamino)methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-67-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[(4-pyridinylamino)methyl]-, (4-ethylphenyl)methyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 455265-68-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloro-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & \\ & & & & & & & \\ \text{Ph-CH}_2-\text{O-C} & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ \end{array}$$

RN 455265-69-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3,4-dihydro-3-oxopyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-70-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[(dimethylamino)methyl]-4-pyridinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-71-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-chloro-4-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

RN 455265-72-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-hydroxy-4-[(4-pyridinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{OH} \\ \hline \\ \text{Ph-CH}_2-\text{O-C} \\ \hline \\ \text{O} \end{array}$$

RN 455265-73-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-chloro-6-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-74-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-75-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
Me & & \\
N & C - O - CH_2
\end{array}$$

RN 455265-76-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridazinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$O$$

$$CH_2-NH$$

$$N$$

$$N$$

RN 455265-77-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-chloro-4-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$CH_2-NH$$

$$CH_2-NH$$

$$C1$$

RN 455265-78-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-bromo-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-79-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(6-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-80-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-81-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-amino-6-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-82-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridazinylamino)methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-83-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-chloro-5-fluoro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-84-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C$$

$$O$$

$$Ph-CH_2-O-C$$

$$O$$

$$Ph-CH_2-O-C$$

$$O$$

RN 455265-85-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-cyclopropylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-86-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ \text{Ph-CH}_2-\text{CH}_2-\text{S} \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-88-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-hydroxy-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-89-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455265-90-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-91-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[1-(4-pyridinylamino)ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-94-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455265-95-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-fluoro-2-pyrimidinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
F & O & O \\
N & NH-CH_2
\end{array}$$

RN 455265-98-2 CAPLUS

CN 4-Piperidinemethanamine, N-(4-methyl-2-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455265-99-3 CAPLUS

CN 4-Piperidinemethanamine, N-(3-methylpyrazinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455266-00-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-methylphenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 455266-01-0 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-fluorophenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & \parallel \\
 & S - CH_2 - CH_2
\end{array}$$

RN 455266-03-2 CAPLUS

CN 4-Pyrimidinecarboxamide, 2-[[[1-[(2-phenylethyl)sulfonyl]-4-piperidinyl]methyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ | & C \\ | & C \\ | & N \end{array}$$

$$\begin{array}{c|c} O & \\ | & C \\ | & C \\ | & N \end{array}$$

$$\begin{array}{c|c} O & \\ | & C \\ | & C \\ | & N \end{array}$$

RN 455266-04-3 CAPLUS

CN 4-Piperidinemethanamine, N-(3-chloropyrazinyl)-1-[(2-phenylethyl)sulfonyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 \\ CH_2 - NH - NH \\ N \end{array}$$

RN 455266-05-4 CAPLUS

CN 4-Piperidinemethanamine, N-(5-methyl-4-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2\text{-}\text{CH}_2\text{-}\text{S} & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-06-5 CAPLUS

CN 4-Piperidinemethanamine, N-(4-amino-5-fluoro-2-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

F
$$N$$
 $NH-CH_2$
 $NH-CH_2$
 $NH-CH_2$
 $NH-CH_2$
 $NH-CH_2$
 $NH-CH_2$
 $NH-CH_2$
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 $NH-CH_2$

RN 455266-07-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2-fluorophenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O & F \\
 & \parallel & \\
 & N & NH-CH_2 & N-CH_2-CH_2
\end{array}$$

RN 455266-08-7 CAPLUS

CN 4-Piperidinemethanamine, N-(6-amino-5-nitro-2-pyridinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & \\ \text{NH2} & & & & & & & \\ \text{O}_{2}\text{N} & & & & & & \\ \text{N} & & & & & & \\ \text{N} & & & & & & \\ \text{NH-} & \text{CH}_{2} & & & & \\ \end{array}$$

RN 455266-11-2 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-pyrazinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{CH}_2-\text{S} & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-12-3 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-4-pyrimidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2\text{-CH}_2\text{-} & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-14-5 CAPLUS

CN 4-Piperidinemethanamine, N-(4-amino-2-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455266-15-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-chlorophenyl)ethyl]sulfonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

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RN 455266-22-5 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylcyclopropyl)carbonyl]-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CH_2-NH & N \\ \hline \\ Ph & N & N \\ \end{array}$$

RN 455266-25-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[1-oxo-4-(2-thienyl)butyl]-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

RN 455266-26-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, 3-thienylmethyl ester (9CI) (CA INDEX NAME)

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RN 455266-28-1 CAPLUS

CN 4-Piperidinemethanamine, 1-(1-oxo-3-phenylpropyl)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2\text{-CH}_2\text{-C} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455266-29-2 CAPLUS

CN 1-Piperidinecarboximidamide, N-cyano-N'-(phenylmethyl)-4-[(4-pyridinylamino)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph-CH}_2-\text{N-C} \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 455266-30-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloropyrazinyl)amino]methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
C1 & & & \\
N & & & \\
N & & & \\
N & & & \\
\end{array}$$

$$\begin{array}{c|c}
N & & & \\
C & & & \\
\end{array}$$

$$\begin{array}{c|c}
C1 & & \\
N & & \\
\end{array}$$

RN 455266-31-6 CAPLUS

CN 1-Piperidinecarboxamide, 4-[[(3-chloropyrazinyl)amino]methyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & \\ & & & & & & \\ Ph-CH_2-NH-C & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ \end{array}$$

RN 455266-32-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[6-(aminomethyl)pyrazinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$H_2N-CH_2$$
 $C-O-CH_2-PH$
 N
 N
 $N+CH_2$

RN 455266-33-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[3-(1-methylethoxy)pyrazinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O \\
C - O - CH_2 - Ph \\
N \\
N \\
OPr-i
\end{array}$$

RN 455266-34-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloropyrazinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455266-35-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-cyanopyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-36-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methoxypyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-37-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methoxypyrazinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

OMe
$$NH-CH_2$$
 $N-C-O-CH_2$ $N-C-O-CH_2$

RN 455266-40-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloropyrazinyl)amino]methyl]-, 2,3-dihydro-1H-inden-2-yl ester (9CI) (CA INDEX NAME)

RN 455266-41-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[3-(aminomethyl)pyrazinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

 $_{\text{H}_2\text{N}-\text{CH}_2}$

RN 455266-42-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-ethoxypyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-43-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-cyano-3-methoxypyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-44-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methoxy-5-methylpyrazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Me NH-CH₂
$$\sim$$
 N \sim O \sim C-O-CH₂-Ph

RN 455266-45-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-fluoro-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-46-3 CAPLUS

CN 4-Piperidinemethanamine, N-(3-methoxypyrazinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-47-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-methoxy-5-methylpyrazinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

RN 455266-48-5 CAPLUS

CN l-Piperidinecarboxylic acid, 4-[[(4,5-dimethyl-2-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Me NH-
$$CH_2$$
 C - O - CH_2 - Ph

RN 455266-50-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-(2-fluorophenyl)cyclopropyl]carbony 1]-N-(3-methoxypyrazinyl)- (9CI) (CA INDEX NAME)

RN 455266-51-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(4,5-dimethyl-2-pyrimidinyl)amino]methyl]-, (4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

Me NH-CH₂ NH-CH₂
$$\stackrel{O}{\parallel}$$
 NH-CH₂ $\stackrel{N}{\parallel}$ NH-CH₂ $\stackrel{N}{\parallel}$

RN 455266-52-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(4-methyl-2-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-53-2 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-(2,6-difluorophenyl)cyclopropyl]car bonyl]-N-(3-methoxypyrazinyl)- (9CI) (CA INDEX NAME)

RN 455266-54-3 CAPLUS

CN 4-Piperidinemethanamine, N-(5-cyano-3-methoxypyrazinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-55-4 CAPLUS

Absolute stereochemistry.

RN 455266-56-5 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-(2,6-difluorophenyl)cyclopropyl]car bonyl]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 455266-57-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-(2,3-difluorophenyl)cyclopropyl]car bonyl]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-58-7 CAPLUS

CN 4-Piperidinemethanamine, N-(5-methyl-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-60-1 CAPLUS

CN 4-Piperidinemethanamine, N-(4,5-dimethyl-2-pyrimidinyl)-1-[[(1R,2R)-2-(2-fluorophenyl)cyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 455266-61-2 CAPLUS

CN 4-Piperidinemethanamine, N-(3-methoxy-5-methylpyrazinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-62-3 CAPLUS

CN 4-Piperidinemethanamine, 4-fluoro-N-(5-methyl-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-63-4 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-(2,6-difluorophenyl)cyclopropyl]car bonyl]-N-(4,5-dimethyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 455266-64-5 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2-fluorophenyl)cyclopropyl]carbonyl]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 455266-65-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2,6-difluorophenyl)cyclopropyl]carbonyl]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
F & O \\
C & N
\end{array}$$

$$\begin{array}{c|c}
CH_2 - NH & N \\
F & O \\
N & O \\
N & O \\
F & O \\
N & O \\
F & O \\
N & O \\
F & O \\
N & O \\
N & O \\
F & O \\
N & O \\
N$$

RN 455266-67-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2,3-difluorophenyl)cyclopropyl]carbonyl]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & C \\
 & N
\end{array}$$

$$\begin{array}{c|c}
 & CH_2-NH \\
 & N \\
 & N
\end{array}$$

$$\begin{array}{c|c}
 & F \\
\end{array}$$

RN 455266-68-9 CAPLUS

CN 4-Piperidinemethanamine, N-(5-fluoro-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 455266-69-0 CAPLUS

CN 4-Piperidinemethanamine, N-(4,5-dimethyl-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-70-3 CAPLUS

CN 4-Piperidinemethanamine, N-(5-bromo-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-71-4 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]-N-[5-[(trimethylsilyl)ethynyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$C = C - SiMe3$$

$$Ph$$

$$R$$

$$O$$

RN 455266-72-5 CAPLUS

CN 4-Piperidinemethanamine, N-(5-ethyl-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-73-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-methylphenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{CH}_2\text{-NH} & \text{N} \\ \hline \\ \text{C} & \text{N} & \text{N} & \text{N} \end{array}$$

RN 455266-74-7 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-fluorophenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\stackrel{\circ}{ } \stackrel{\circ}{ } \stackrel{\circ}$$

RN 455266-75-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(3-fluorophenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 455266-76-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2,6-difluorophenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
F & O \\
C & N
\end{array}$$

$$\begin{array}{c|c}
CH_2 - NH & N \\
N & N
\end{array}$$

RN 455266-78-1 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2,3-difluorophenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 455266-79-2 CAPLUS

CN 4-Piperidinemethanamine, N-(5-ethynyl-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-80-5 CAPLUS

CN 4-Piperidinemethanamine, N-[5-(cyclopropylethynyl)-2-pyrimidinyl]-1[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 455266-81-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2-methylphenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & CH_2-NH-N \\ \hline \\ C & N & N \end{array}$$

RN 455266-82-7 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(4-chlorophenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 455266-83-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2-methoxyphenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & \text{O} \\ \hline \\ \text{C} & \text{N} \end{array}$$

RN 455266-84-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2,4-difluorophenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F & O & CH_2-NH & N \\ \hline & C & N & N \\ \end{array}$$

RN 455266-85-0 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(3-methylphenyl)cyclopropyl]carbonyl]-N-(5-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

$$\bigcap_{Me} CH_2-NH - \bigcap_{N} Me$$

RN 455266-86-1 CAPLUS

CN 4-Piperidinemethanamine, N-(5-cyano-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-87-2 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]-N-[5-(phenylethynyl)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-88-3 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(3-methylphenyl)cyclopropyl]carbonyl]-N-2-

pyrimidinyl- (9CI) (CA INDEX NAME)

RN 455266-89-4 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(3-chlorophenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ \end{array}$$

RN 455266-91-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(3-methoxyphenyl)cyclopropyl]carbonyl]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CH_2-NH-N \\ \hline \\ MeO & N \end{array}$$

RN 455266-92-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2-methylphenyl)cyclopropyl]carbonyl]-N-(5-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & CH_2-NH & N \\ \hline \\ C & N & N \end{array}$$

RN 455266-93-0 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2-fluorophenyl)cyclopropyl]carbonyl]-N-(5-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 455266-94-1 CAPLUS

CN 4-Piperidinemethanamine, N-(5-fluoro-2-pyrimidinyl)-1-[[2-(pentafluorophenyl)cyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 455266-95-2 CAPLUS

CN 4-Piperidinemethanamine, N-(3-fluoro-2-pyridinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455266-96-3 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2,3-difluorophenyl)cyclopropyl]carbonyl]-N-(5-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
C & C & C & N \\
\hline
C & N & M \\
\hline
C & N & M \\
\end{array}$$

RN 455266-97-4 CAPLUS

CN 4-Piperidinemethanamine, N-(5-fluoro-2-pyrimidinyl)-1-[[2-(2-methylphenyl)cyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 455266-98-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-chloropyrazinyl)amino]methyl]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
C1 & N - C - O - CH_2
\end{array}$$

$$N - C - O - CH_2$$

RN 455266-99-6 CAPLUS

CN 4-Piperidinemethanamine, 1-[[2-(2,6-difluorophenyl)cyclopropyl]carbonyl]-N-(5-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
F & O \\
C & N
\end{array}$$

$$\begin{array}{c|c}
CH_2 - NH & N \\
N & Me$$

RN 455267-00-2 CAPLUS

CN 4-Piperidinemethanamine, N-(5-fluoro-2-pyrimidinyl)-1-[[2-(3-methylphenyl)cyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ & & \\ \end{array}$$

RN 455267-02-4 CAPLUS

CN 4-Piperidinemethanamine, N-(4-methyl-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455267-03-5 CAPLUS

CN 4-Piperidinemethanamine, N-(5-methyl-2-pyrimidinyl)-1-[[2-(5-methyl-2-thienyl)cyclopropyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 455268-07-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)methyl]-, (3-fluorophenyl)methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455265-53-9 CMF C19 H22 F N3 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455290-06-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-2-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455290-08-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-chloro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455290-10-5 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1S,2S)-2-(2-fluorophenyl)cyclopropyl]carbony 1]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455290-13-8 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1S,2S)-2-(2,3-difluorophenyl)cyclopropyl]car bonyl]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455305-07-4 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1S,2S)-2-(2,6-difluorophenyl)cyclopropyl]car bonyl]-N-(5-fluoro-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

IT 455267-18-2P 455267-68-2P 455267-73-9P 455267-78-4P 455267-93-3P 455267-94-4P 455267-96-6P 455267-98-8P 455267-99-9P 455268-00-5P 455268-01-6P 455268-04-9P 455268-05-0P 455268-06-1P 455290-15-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-acyl-4-(heterocyclylaminomethyl) piperidines as NMDA/NR2B antagonists)

RN 455267-18-2 CAPLUS

CN 4-Piperidinemethanamine, N-(2-chloro-5-methyl-4-pyrimidinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

C1
$$S-CH_2-CH_2-Ph$$
 $S-CH_2-CH_2-Ph$ O S

RN 455267-68-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-fluoro-4-pyridinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph-CH}_2-\text{O-C} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 455267-73-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-chloro-5-methyl-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455267-78-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5,6-dichloro-4-pyridazinyl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$N$$
 $NH-CH_2$
 $C-O-CH_2-PH$
 C

RN 455267-93-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-chloro-4-pyrimidinyl)amino]methyl]-, phenylmethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 455267-94-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-hydroxy-4-[(4-pyridinylamino)methyl]-, phenylmethyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 455265-72-2 CMF C19 H23 N3 O3

$$\begin{array}{c|c} \text{OH} & \text{OH} \\ \hline \\ \text{Ph-CH}_2\text{-O-C} \\ \parallel \\ \text{O} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455267-96-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(3-fluoro-4-pyridinyl)amino]methyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455267-68-2 CMF C19 H22 F N3 O2

$$Ph-CH_2-O-C$$

$$O$$

$$Ph-CH_2-O-C$$

$$O$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455267-98-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[3-(aminomethyl)pyrazinyl]amino]methyl]-,

phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455266-41-8 CMF C19 H25 N5 O2

$$\begin{array}{c|c}
 & O \\
 & C \\$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455267-99-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[6-(aminomethyl)pyrazinyl]amino]methyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455266-32-7 CMF C19 H25 N5 O2

$$\begin{array}{c|c} \mathsf{H_2N-CH_2} & \mathsf{O} \\ \\ \mathsf{N} & \mathsf{NH-CH_2} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455268-00-5 CAPLUS

CN 4-Piperidinemethanamine, N-(5-methyl-2-pyrimidinyl)-1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 455268-01-6 CAPLUS

CN 4-Piperidinemethanamine, 4-fluoro-1-[[(1R,2R)-2-(2-fluorophenyl)cyclopropyl]carbonyl]-N-(5-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 455268-04-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]-N-2-pyrimidinyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455268-03-8 CMF C20 H24 N4 O Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455268-05-0 CAPLUS

CN 4-Piperidinemethanamine, N-[5-(cyclopropylethynyl)-2-pyrimidinyl]-1[[(1R,2R)-2-phenylcyclopropyl]carbonyl]-, mono(trifluoroacetate) (9CI)
(CA INDEX NAME)

CM 1

CRN 455266-80-5 CMF C25 H28 N4 O

Absolute stereochemistry.

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 455268-06-1 CAPLUS

CN 4-Piperidinemethanamine, 1-[[(1R,2R)-2-phenylcyclopropyl]carbonyl]-N-[5-(phenylethynyl)-2-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 455266-87-2 CMF C28 H28 N4 O

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 455290-15-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(5-methyl-4-pyrimidinyl)amino]methyl]-, (4-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

IT 455267-76-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of N-acyl-4-(heterocyclylaminomethyl)piperidines as NMDA/NR2B antagonists)

RN 455267-76-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[5-chloro-2,6-bis(methylthio)-4-pyrimidinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

IT 455267-07-9P 455267-08-0P 455267-15-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-acyl-4-(heterocyclylaminomethyl) piperidines as NMDA/NR2B antagonists)

RN 455267-07-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-hydroxy-4-[[(2,3,5,6-tetrachloro-4-pyridinyl)amino]methyl]-, phenylmethyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$\begin{array}{c|c} C1 & HO & S & N & O \\ \hline & HO & S & N & O \\ \hline & R & & R & \\ \hline & C1 & & C1 & \\ \hline & & & & & \\ \end{array}$$

RN 455267-08-0 CAPLUS

CN 2-Pyridinecarboxylic acid, 4-[[[1-[(phenylmethoxy)carbonyl]-4-piperidinyl]methyl]amino]- (9CI) (CA INDEX NAME)

RN 455267-15-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[[(2,4-dimethoxyphenyl)methyl]amino]-6-methyl-4-pyrimidinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
L11
     2001:115130 CAPLUS
AN
DN
     134:178474
ΤI
     Preparation of oxobenzazepinealkanoates and analogs as integrin receptor
     antagonists
     Kling, Andreas; Geneste, Herve; Lange, Udo; Lauterbach, Arnulf; Graef,
TN
     Claudia Isabella; Subkowski, Thomas; Holzenkamp, Uta; Mack, Helmut;
     Sadowski, Jens; Hornberger, Wilfried; Laux, Volker
     BASF Aktiengesellschaft, Germany
PA
     PCT Int. Appl., 158 pp.
SO
     CODEN: PIXXD2
DT
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LA
     German
FAN.CNT 1
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                                                                  DATE
     PATENT NO.
                                           ______
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                                                                   _____
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                                20010215
                                           WO 2000-EP7440
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     WO 2001010847
                        - A3
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             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
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         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                          DE 1999-19936780
     DE 19936780
                         A1
                                20010215
                                                                   19990809
     CA 2379977
                         AΑ
                                20010215
                                           CA 2000-2379977
                                                                   20000801
                         A2
                                20020508
                                           EP 2000-958347
                                                                   20000801
     EP 1202988
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             IE, SI, LT, LV, FI, RO, MK, CY, AL
     BR 2000013265
                         Α
                                20020514
                                           BR 2000-13265
                                                                   20000801
     TR 200200357
                         Т2
                                20020923
                                           TR 2002-200200357
                                                                   20000801
     JP 2003506441
                         T2
                                20030218
                                           JP 2001-515313
                                                                   20000801
                               20021229
                                           BG 2002-106395
                                                                   20020206
     BG 106395
                         Α
                                           NO 2002-644
     NO 2002000644
                        Α
                                20020318
                                                                   20020208
PRAI DE 1999-19936780
                        Α
                                19990809
     WO 2000-EP7440
                         W
                                20000801
OS
     MARPAT 134:178474
     RZZ1R1 [I; R = group contg, ≥1 non-H H-bonding atom; R1 = CO2H, or
AB
     group hydrolizable to CO2H; Z = e.g., (hetero)annelated
     2-oxo-1-benzazepin-1,5-diyl; Z1 = bond, (un)substituted NHCH2, -OCH2,
     -alkylene, -CH:CH, etc.] were prepared Thus, Me 11-methoxycarbonylmethyl-6-
     oxo-6,11-dihydro-5H-dibenz[b,e]azepine-5-acetate (preparation given) was
     amidated by N-(2-aminoethyl)pyridine-2-amine to give, after saponification,
title
     compound II. Data for biol. activity of I were given.
IT
     326399-42-2P 326401-50-7P 326401-54-1P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of oxobenzazepinealkanoates and analogs as integrin receptor
        antagonists)
RN
     326399-42-2 CAPLUS
     5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[(2-
     pyridinylamino)methyl]-1-piperidinyl]ethyl]-, monoacetate (9CI) (CA INDEX
     NAME)
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CM 1

CRN 326399-41-1 CMF C29 H30 N4 O4

PAGE 1-A

PAGE 2-A

CM 2.

CRN 64-19-7 CMF C2 H4 O2

RN 326401-50-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[2-(2-pyridinylamino)ethyl]-1-piperidinyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

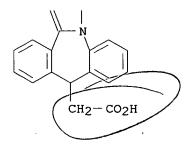
PAGE 2-A

RN 326401-54-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[2-(2-pyridinylamino)ethyl]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A



```
ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
L11
     2001:12267 CAPLUS
AN
     134:71602
DN
ΤI
     Preparation and effect of benzimidazolylpyrimidine derivatives as SRC
     kinase inhibitors
     Goulet, Joung L.; Holmes, Mark A.; Hunt, Julianne A.; Mills, Sander G.;
TN
     Parsons, William H.; Sinclair, Peter J.; Zaller, Dennis M.
     Merck & Co., Inc., USA
PA
     PCT Int. Appl., 173 pp.
SO
     CODEN: PIXXD2
DТ
     Patent
     English
LA
FAN.CNT 1
                                                                   DATE
     PATENT NO.
                         KIND
                                DATE
                                           APPLICATION NO.
                         ____
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                                20010104 WO 2000-US17510
                                                                   20000626
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             HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU,
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             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                           CA 2000-2376957
                                                                   20000626
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                                20010104
     US 6329380
                          В1
                                20011211
                                            US 2000-603688
                                                                   20000626
     EP 1206260
                         A1
                                20020522
                                           EP 2000-953637
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            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
                          Т2
                                20030128
                                            JP 2001-505916
                                                                   20000626
     JP 2003503351
                          Р
                                19990630
PRAI US 1999-141630P
     WO 2000-US17510
                          W
                                20000626
OS
     MARPAT 134:71602
     Title Pyrimidine compds. [I; R1, R2 independently = H, Br, C1, I, F, OH,
AΒ
     SH, CN, NO2, NH2; R1R2; fused methylenedioxy ring, fused 6-membered aromatic
     ring; R3, R5 independently = H, alkyl, aryl; R3R5 = O; R4 = H, alkyl,
     alkoxyl; X1, X2, X3, X4 independently = CH, CBr, COH, CSH, CNO2, N; R7 =
     H, NH2, alkyl, aryl, alkylamino, arylamino; Y = O, N, CH; Z = CO, SO2,
     bond; m, n independently = 0, 1, 2, 3, 4], or their pharmaceutically
     acceptable salts, hydrates, solvates, crystal forms and individual
     diastereomers, and pharmaceutical compns. including the same, which are
     inhibitors of tyrosine kinase enzymes, and as such are useful in the
     prophylaxis and treatment of protein tyrosine kinase-associated disorders,
     such as immune diseases, hyperproliferative disorders and other diseases
     in which inappropriate protein kinase action is believed to play a role,
     such as cancer, angiogenesis, atherosclerosis, graft rejection, rheumatoid
     arthritis and psoriasis. Thus, the title compound II was prepared and tested.
     315717-01-2P 315717-13-6P 315717-22-7P
IT
     315717-24-9P 315717-39-6P 315719-53-0P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation and effect of benzimidazolylpyrimidine derivs. as SRC kinase
        inhibitors)
RN
     315717-01-2 CAPLUS
     1-Piperidinecarboxylic acid, 3-[[[4-(1H-benzimidazol-1-yl)-2-
```

pyrimidinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN

1-Piperidinecarboxylic acid, 3-[1-[[4-(1H-benzimidazol-1-yl)-2pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 315/17-22-7 CAPLUS 3-Piperidinemethanamine, N-[4-(1H-benzimidazol-1-yl)-2-pyrimidinyl]-CN α -methyl-1-(phenylacetyl)- (9CI) (CA INDEX NAME)

315717-24-9 CAPLUS 1-Piperidinecarboxylic acid, 3-[1-[[4-(1H-benzimidazol-1-yl)-2pyrimidinyl]amino]ethyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 315717-39-6 CAPLUS

1-Piperidinecarboxylic acid, 4-[[[4-(1H-benzimidazol-1-yl)-2-CN pyrimidinyl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & C \\
 & C \\
 & O \\$$

RN 315719-53-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 2-[1-[[4-(1H-benzimidazol-1-yl)-2-pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

IT 315717-82-9P 315717-84-1P 315717-87-4P

315717-89-6P, 2-[1-(1-Benzyloxycarbonylpiperidin-3-yl)ethylamino]-4-[5-N-(tert-butyloxycarbonyl)aminobenzimidazol-1-yl]pyrimidine

315718-00-4P 315718-02-6P 315718-03-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and effect of benzimidazolylpyrimidine derivs. as SRC kinase inhibitors)

RN 315717-82-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[1-[[4-[5-(benzoylamino)-1H-benzimidazol-1-yl]-2-pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 315717-84-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[1-[[4-[5-[(2,2-dimethyl-1-oxopropyl)amino]-1H-benzimidazol-1-yl]-2-pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 315717-87-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[1-[[4-(1H-benzimidazol-1-yl)-2-pyrimidinyl]amino]ethyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

RN 315717-89-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[1-[[4-[5-[[(1,1-dimethylethoxy)carbonyl]amino]-1H-benzimidazol-1-yl]-2-pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 315718-00-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[1-[[4-[5-(4-pyridinyl)-1H-benzimidazol-1-yl]-2-pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 315718-02-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[1-[[4-(3H-imidazo[4,5-c]pyridin-3-yl)-2-pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 315718-03-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[1-[[4-(1H-imidazo[4,5-c]pyridin-1-yl)-2-pyrimidinyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1987:515499 CAPLUS

DN 107:115499

TI Preparation of (pyridylcarbamoyl)piperidine derivatives as cardiovascular agents and antihypertensives

IN Muro, Tomio; Seki, Toshio; Kawakami, Minoru; Inui, Atsushi; Sato, Hiroyuki

PA Yoshitomi Pharmaceutical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 12 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	KIND DATE	APPLICATION NO.	DATE		
		-				
PI JP 62089679	A2	19870424	JP 1986-139474	19860616		
JP 06080054	В4	19941012				
PRAI JP 1985-13360	6 A1	19850619				

OS CASREACT 107:115499

The title compds. [I; R1 = H, OH, alkoxy, alkoxycarbonyloxy, alkanoyloxy, aralkyloxycarbonyloxy; R2 = H, alkyl, aralkyl, dialkylaminoalkyl; R3, R4 = H, halo, alkyl, aralkyloxy; Z = O, S, H2; L = H, alkyl, dialkylaminoalkyl, tetrahydrofurfuryl, carbamoylalkyl, phthalimidoalkyl, acyl, (un)substituted phenoxy(hydroxy)alkyl, (un)substituted benzoylalkyl, (un)substituted phenylalkyl, etc.] and their acid addition salts, useful as antihypertensives and cardiovascular agents (no data), were prepared A mixture of 7.34 g 4-(4-pyridylcarbamoyl)piperidine.2HBr and 4.93 g 1-(2, 3-epoxypropyloxy)-2-(thienylmethyl)benzene in EtOH containing Et3N was refluxed for 10 h to give the piperidine derivative II.

IT 110105-87-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as cardiovascular agent)

RN 110105-87-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pyridinylamino)thioxomethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

10/079,452 (RCE)

=> => d his

(FILE 'HOME' ENTERED AT 13:47:33 ON 21 JAN 2005)

	FILE	'REGISTRY' ENTERED AT 13:49:13 ON 21 JAN 2005
L1		SCREEN 1840
L2		SCREEN 2016 OR 2039 OR 2040 OR 2045 OR 2047
L3		STRUCTURE UPLOADED
L4		QUE L3 AND L1 NOT L2
L5	•	5 S L4 SSS SAM
L6		231 S L4 SSS FUL
L7		STRUCTURE UPLOADED
L8		4 S L7 SSS SAM SUB=L6
L9		24 S L7 SSS FUL SUB=L6
L10		207-S L6 NOT L9

FILE 'CAPLUS' ENTERED AT 13:56:00 ON 21 JAN 2005 L11 7 S L10

FILE 'CAOLD' ENTERED AT 13:57:09 ON 21 JAN 2005

=> s 110

L12 0 L10

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.43	240.22
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY 0.00	SESSION -5.11

STN INTERNATIONAL LOGOFF AT 13:57:22 ON 21 JAN 2005

```
C:\Program Files\Stnexp\Queries\10079452
chain nodes :
    7
      8 9 10
                  11
                       14
                            15
                                19
                                     20
                                         21
                                              22
                                                  23
                                                       27
                                                           29
                                                                30
                                                                    31
                                                                         32
                                                                             35
                                                                                  36
                                                                                      37
```

```
47 48
    46
                157
ring nodes :
                5
                   6
                      16 17
                              18
                                   51
                                       52
                                           53 54
                                                    55
                                                        56
                                                             57
                                                                 58
                                                                    59
    1
                                                              76 77 78 79
            64
                    66
                         67
                             68 69 70
                                         71
                                              72
                                                  73 74 75
       63
                65
            90
                91
                    92
                         93
                             94
                                 95
                                     96
                                          97
                                              98
                                                  99
                                                      100 101
                                                                 102
                                                                      103
                                                                           104
    105
         106
              107
                   108
                         109
                              110
                                   111
                                         112
                                              113
                                                  114
                                                        115
                                                              116
                                                                   117
                                                                        125
                                                                             126
              129
                         131
                                              135
                                                   136
                                                        137
                                                              138
                                                                   139
                                                                        140
    127
         128
                   130
                              132
                                   133
                                         134
                                         149
                                              150
                                                   151
    142
         143
              144
                   145
                         146
                              147
                                   148
chain bonds :
              7-9 9-10
                         10-11
                                 14-15
                                         14-18 16-19 20-21
                                                                20-22
                                                                       22-23
    2-46 7-8
          27-30 30-31
                                 35-36 36-37 47-48 48-157
    27-29
                          31-32
ring bonds :
    1-2 1-6
              2-3
                   3 - 4
                         4-5
                             5-6
                                  16-17
                                          16-18 17-18
                                                        51-52
                                                                51-55
                                                                       52-53
                  56-57
                                 57-58
                                        58-59
                                               59-60
                                                       61-62
                                                               61-65
                                                                      62-63
                                                                             63-64
    53-54
           54-55
                          56-60
                                                                      73-74
                                                               72-73
                                                                             74 - 75
                  66-70
                                         69-70
                                                71-72
                                                       71-75
    64 - 65
           66-67
                          67-68
                                 68-69
                  77-78
                          78-79
                                                       89-90
           76-80
                                 79-80
                                                88-92
                                                                      91-92
                                                                             93 - 94
    76-77
                                         88-89
                                                               90-91
    93-97
           94 - 95
                          96-97
                                 98-99
                                         98-102 99-100 100-101 101-102
                  95-96
    103-104
             103-107
                       104-105
                                105-106
                                         106-107
                                                   108-109
                                                            108-112
                                          114-115
                                                   115-116
                                                             116-117
    110-111
             111-112
                       113-114
                                113-117
    125-130
             126-127
                       127-128
                                128-129
                                          129-130
                                                   129-131
                                                             130-133
                                                                      131-132
    132-133
             134-135
                       134-139
                                135-136
                                          136-137
                                                   137-138
                                                            138-139
                                                                      138-140
    139-142
             140-141
                       141-142
                                143-144
                                          143-148
                                                   144-145
                                                             145-146
                                                                      146-147
    147-148
                       148-151
                                149-150
                                          150-151
             147-149
exact/norm bonds :
    1-2 1-6 2-3 2-46
                          3-4 4-5 5-6
                                         7-8 7-9 10-11
                                                           14-15
                                                                  16-19
                                                                          20-21
    22-23
           27-29
                  27-30
                          36-37
                                 47-48
                                         48-157 54-55 59-60 64-65
                                                                       68-69
    69-70
           73-74
                  74 - 75
                          78-79
                                 79-80
                                         88-89 88-92 89-90 90-91
                                                                      91-92
                                                                            93-94
                                         98-102 99-100 100-101 101-102
    93-97
           94-95
                  95-96
                          96-97
                                 98-99
                                         106-107
    103-104
             103-107
                                105-106
                                                                      109-110
                      104-105
                                                   108-109
                                                            108-112
                                                   115-116
    110-111
                       113-114
                                          114-115
                                                             116-117
             111-112
                                113-117
                                                                      129-130
    129-131
             130-133
                       131-132
                                132-133
                                          138-139
                                                   138-140
                                                             139-142
                                                                      140-141
    141-142
             147-148
                       147-149
                                148-151
                                         149-150
                                                   150-151
exact bonds :
```

```
9-10 14-18 16-17 16-18 17-18
                                     20-22 30-31 31-32
                                                         35-36 51-52 51-55
    52-53 53-54 56-57
                              57-58 58-59 61-62
                                                   61-65
                        56-60
                                                         62-63
                                                                63-64 66-67
    66-70
          67-68
                 71-72
                        71-75
                               72-73
                                      76-77
                                            76-80
                                                   77-78
                                                          125-126
                                                                  125-130
                                              135-136 136-137
    126-127 127-128
                     128-129
                              134-135
                                      134-139
                                                                 137-138
                              145-146
                                      146-147
    143~144
            143-148
                     144-145
isolated ring systems :
    containing 1 : 16 : 51 : 56 : 61 : 66 : 71 : 76 : 88 : 93 : 98 : 103 : 108 :
    113 : 125 : 134 : 143 :
G1:0,N
G2: [*1], [*2], [*3], [*4], [*5]
G3:[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16],[*17],[*18],[*19
    ],[*20]
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom
                                                  7:CLASS
                                                           8:CLASS
                                                                    9:CLASS
    10:CLASS
             11:Atom 14:CLASS 15:CLASS 16:Atom
                                                  17:Atom
                                                           18:Atom
                                                                    19:Atom
                                23:Atom
36:CLASS
    20:CLASS
             21:CLASS
                       22:CLASS
                                         27:CLASS 29:CLASS 30:CLASS
             32:Atom 35:CLASS 50:CLASS 51:Atom
    31:CLASS
                                         37:Atom 46:CLASS
                                                           47:CLASS
                               52:Atom 53:Atom 54:CLASS
    48:CLASS
                                                          58:Atom 59:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:CLASS
    57:Atom
            66:CLASS 67:CLASS 68:Atom 69:CLASS
    65:Atom
                                                  70:CLASS
                                                            71:CLASS
                                75:CLASS 76:CLASS
                      74:CLASS
   72:CLASS
            73:Atom
                                                  77:CLASS
                                                             78:Atom
    79:CLASS
             80:CLASS
                      88:Atom 89:CLASS 90:CLASS 91:Atom 92:Atom
                                                                     93:Atom
                       96:Atom 97:Atom 98:Atom 99:CLASS
    94:CLASS
             95:CLASS
                                                           100:CLASS
    101:Atom
             102:Atom
                       103:Atom 104:CLASS 105:CLASS
                                                     106:Atom 107:Atom
   108:Atom
             109:CLASS
                        110:CLASS 111:Atom 112:Atom
                                                      113:Atom 114:CLASS
   115:CLASS
             116:Atom
                        117:Atom 125:Atom 126:Atom 127:Atom 128:Atom
   129:Atom
             130:Atom 131:Atom 132:Atom
                                          133:Atom 134:Atom 135:Atom
   136:Atom.
             137:Atom 138:Atom 139:Atom
                                          140:Atom 141:Atom
                                                             142:Atom
    143:Atom
             144:Atom 145:Atom 146:Atom
                                          147:Atom 148:Atom
                                                             149:Atom
   150:Atom
             151:Atom 157:CLASS
Generic attributes :
    11:
   Saturation
                         : Unsaturated
   19:
   Saturation
                          : Unsaturated
   23:
   Saturation
                          : Unsaturated
   32:
   Saturation
                          : Unsaturated
   37:
   Saturation
                         : Unsaturated
```

Element Count :
Node 47: Limited
C,C1-5

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1840

CyCH292-4

=>

L1 SCREEN CREATED

=> screen 2016 OR 2039 OR 2040 OR 2045 OR 2047

L2 SCREEN CREATED

37363%

chain nodes : 7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47 48 81 92 ring nodes : 1 2 3 4 5 6 16 17 18 51 52 53 54 55 56 57 58 59 60 61 62 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 chain bonds : $2-46 \quad 7-8 \quad 7-9 \quad 9-10 \quad 10-11 \quad 14-15 \quad 14-18 \quad 16-19 \quad 20-21 \quad 20-22 \quad 22-23 \quad 27-29 \quad 27-30$ 30-31 31-32 35-36 36-37 47-48 48-92 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 51-52 51-55 52-53 53-54 54-55 56-57 56-60 57-58 58-59 59-60 61-62 61-65 62-63 63-64 64-65 66-67 66-70 67-68 68-69 69-70 71-72 71-75 72-73 73-74 74-75 76-77 76-80 77-78 78-79 79-80 exact/norm bonds : 1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 10-11 14-15 16-19 20-21 22-23 27-29 27-30 36-37 47-48 48-92 54-55 59-60 64-65 68-69 69-70 73-74 74-75 78-79 79-80

10/079,452 (RCE)

```
exact bonds :
9-10 14-18 16-17 16-18 17-18 20-22 30-31 31-32 35-36 51-52 51-55 52-53
53-54 56-57 56-60 57-58 58-59 61-62 61-65 62-63 63-64 66-67 66-70 67-68
71-72 71-75 72-73 76-77 76-80 77-78
isolated ring systems :
containing 1 : 16 : 51 : 56 : 61 : 66 : 71 : 76 :
G1:0,N
G2: [*1], [*2], [*3], [*4], [*5]
G3: [*6], [*7], [*8], [*9], [*10], [*11], [*12]
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
         22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom
35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom
52:Atom 53:Atom 54:CLASS 55:Atom 56:Atom 57:Atom 58:Atom 59:CLASS 60:Atom
61:Atom 62:Atom 63:Atom 64:CLASS 65:Atom 66:CLASS 67:CLASS 68:Atom 69:CLASS
70:CLASS 71:CLASS 72:CLASS 73:Atom 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:Atom 79:CLASS 80:CLASS 81:Atom 92:CLASS
Generic attributes :
11:
Saturation
                     : Unsaturated
19:
Saturation
                     : Unsaturated
23:
Saturation
                     : Unsaturated
32:
Saturation
                     : Unsaturated
37:
Saturation
                     : Unsaturated
81:
Saturation
                     : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System
                   : Monocyclic
Element Count :
Node 47: Limited
   C, C1-5
Node 81: Limited
   C,C2
   N,N2
   S,S1
   0,00
```

L3 STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4 QUE L3 AND L1 NOT L2

=> d 14

L4 HAS NO ANSWERS

L1 SCR 1840

L2 SCR 2016 OR 2039 OR 2040 OR 2045 OR 2047

L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L4 QUE L3 AND L1 NOT L2

=> s 14 sss sam

SAMPLE SEARCH INITIATED 14:53:01 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 27013 TO ITERATE

3.7% PROCESSED

1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **INCOMPLETE**

BATCH . **COMPLETE**

PROJECTED ITERATIONS:

530433 TO 550087

PROJECTED ANSWERS:

0 TO

.

L5

0 SEA SSS SAM L3 AND L1 NOT L2

=>

Uploading C:\Program Files\Stnexp\Queries\10079452 (rce12).str

```
chain nodes :
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47
48 89
ring nodes :
1 2 3 4 5 6 16 17 18 51 52 53 54 55 56 57 58 59 60 61 62
64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80
chain bonds :
2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30
30-31 31-32 35-36 36-37 47-48 48-89
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 51-52 51-55 52-53 53-54
54-55 56-57 56-60 57-58 58-59 59-60 61-62 61-65 62-63 63-64 64-65 66-67
66-70 67-68 68-69 69-70 71-72 71-75 72-73 73-74 74-75 76-77 76-80 77-78
78-79 79-80
exact/norm bonds :
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 10-11 14-15 16-19 20-21 22-23
27-29 27-30 36-37 47-48 48-89 54-55 59-60 64-65 68-69 69-70 73-74 74-75
78-79 79-80
exact bonds :
71-72 71-75 72-73 76-77 76-80 77-78
isolated ring systems :
containing 1 : 16 : 51 : 56 : 61 : 66 : 71 : 76 :
G1:0,N
G2:[*1],[*2],[*3],[*4],[*5]
G3: [*6], [*7], [*8], [*9], [*10], [*11]
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom
35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom
52:Atom 53:Atom 54:CLASS 55:Atom 56:Atom 57:Atom 58:Atom 59:CLASS 60:Atom
61:Atom 62:Atom 63:Atom 64:CLASS 65:Atom 66:CLASS 67:CLASS 68:Atom 69:CLASS
70:CLASS 71:CLASS 72:CLASS 73:Atom 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:Atom 79:CLASS 80:CLASS 89:CLASS
Generic attributes :
11:
Saturation
                   : Unsaturated
19.
Saturation
                   : Unsaturated
23:
Saturation
                   : Unsaturated
32:
Saturation
                   : Unsaturated
37:
Saturation
                   : Unsaturated
Element Count :
```

Node 47: Limited C,C1-5

L6 STRUCTURE UPLOADED

=> d 16L6 HAS NO ANSWERS STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Structure attributes must be viewed using STN Express query preparation.

=> s 16 sss sam SAMPLE SEARCH INITIATED 14:54:06 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 363 TO ITERATE

100.0% PROCESSED 363 ITERATIONS SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS:

ONLINE **COMPLETE** **COMPLETE** BATCH

8403

PROJECTED ITERATIONS:

6117 TO

PROJECTED ANSWERS:

1 TO

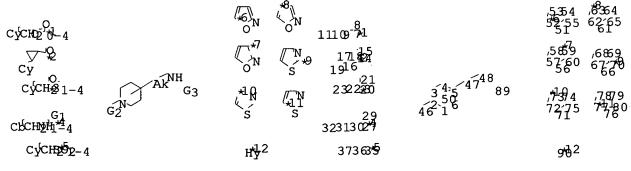
80

L7

1 SEA SSS SAM L6

=> =>

Uploading C:\Program Files\Stnexp\Queries\10079452 (rce13).str



chain nodes :

```
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47
48 89 90
ring nodes :
1 2 3 4 5 6 16 17 18 51 52 53 54 55 56 57 58 59 60 61 62
                                                                           63
64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80
chain bonds :
2-46 7-8 7-9 9-10 10-11 14-15
                                  14-18
                                        16-19 20-21 20-22 22-23 27-29 27-30
30-31 31-32 35-36 36-37 47-48
                                  48-89
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 51-52 51-55 52-53 53-54
54-55 56-57 56-60 57-58 58-59 59-60 61-62 61-65 62-63 63-64 64-65 66-67
66-70 67-68 68-69 69-70 71-72 71-75 72-73 73-74 74-75 76-77 76-80
                                                                          77-78
78-79 79-80
exact/norm bonds :
1-2 \quad 1-6 \quad 2-3 \quad 2-46 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-9 \quad 10-11 \quad 14-15 \quad 16-19 \quad 20-21 \quad 22-23
27-29 27-30 36-37 47-48 48-89 54-55 59-60 64-65 68-69 69-70 73-74 74-75
78-79 79-80
exact bonds :
9-10 14-18 16-17 16-18 17-18 20-22 30-31 31-32 35-36 51-52 51-55 52-53
53-54 56-57 56-60 57-58 58-59 61-62 61-65 62-63 63-64 66-67 66-70 67-68 71-72 71-75 72-73 76-77 76-80 77-78
isolated ring systems :
containing 1 : 16 : 51 : 56 : 61 : 66 : 71 : 76 :
G1:0,N
G2: [*1], [*2], [*3], [*4], [*5]
G3: [*6], [*7], [*8], [*9], [*10], [*11], [*12]
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom
35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom
52:Atom 53:Atom 54:CLASS 55:Atom 56:Atom 57:Atom 58:Atom 59:CLASS 60:Atom
61:Atom 62:Atom 63:Atom 64:CLASS 65:Atom 66:CLASS 67:CLASS 68:Atom 69:CLASS
70:CLASS 71:CLASS 72:CLASS 73:Atom 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:Atom 79:CLASS 80:CLASS 89:CLASS 90:Atom
Generic attributes :
11:
Saturation
                     : Unsaturated
19:
Saturation
                     : Unsaturated
23:
Saturation
                     : Unsaturated
32:
Saturation
                     : Unsaturated
Saturation
                     : Unsaturated
90:
Saturation
                     : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System : Monocyclic
```

Element Count :

Node 47: Limited C,C1-5

Node 90: Limited

C, C2

S, S1

N,N2

0,00

L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

L8

STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 18 sss sam

SAMPLE SEARCH INITIATED 14:57:23 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 29643 TO ITERATE

3.4% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

582569 TO 603151

PROJECTED ANSWERS:

0 TO 0

L9

0 SEA SSS SAM L8

=>

Uploading C:\Program Files\Stnexp\Queries\10079452 (rce14).str

```
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30
                                                       31
                                                          32
                                                               35 36 37 46 47
48 127
ring nodes :
1 2 3 4 5 6 16 17 18 51 52 53 54 55 56 57 58 59 60 61 62 63
64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 88 89 90 91
92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107
                                                                     108 109
110 111 112 113 114 115 116 117
chain bonds :
2 - 46 \quad 7 - 8 \quad 7 - 9 \quad 9 - 10 \quad 10 - 11 \quad 14 - 15 \quad 14 - 18 \quad 16 - 19 \quad 20 - 21 \quad 20 - 22 \quad 22 - 23 \quad 27 - 29 \quad 27 - 30
30-31 31-32 35-36 36-37 47-48 48-127
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 51-52 51-55 52-53 53-54
54-55 56-57 56-60 57-58 58-59 59-60 61-62 61-65 62-63 63-64 64-65 66-67
66-70 67-68 68-69 69-70 71-72 71-75 72-73 73-74 74-75 76-77 76-80 78-79 79-80 88-89 88-92 89-90 90-91 91-92 93-94 93-97 94-95 95-96
                                                                    76-80
98-99 98-102 99-100 100-101 101-102 103-104 103-107 104-105 105-106
106-107 108-109 108-112 109-110 110-111 111-112 113-114 113-117 114-115
115-116 116-117
exact/norm bonds :
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 10-11 14-15 16-19 20-21 22-23
27-29 27-30 36-37 47-48 48-127
                                  54-55 59-60 64-65 68-69 69-70 73-74 74-75
78-79 79-80 88-89 88-92 89-90 90-91 91-92 93-94 93-97 94-95 95-96 96-97
98-99 98-102 99-100 100-101 101-102 103-104 103-107 104-105 105-106
106-107 108-109 108-112 109-110 110-111 111-112 113-114 113-117 114-115
115-116 116-117
exact bonds :
```

chain nodes :

10/079,452 (RCE)

9-10 14-18 16-17 16-18 17-18 20-22 30-31 31-32 35-36 51-52 51-55 52-53 53-54 56-57 56-60 57-58 58-59 61-62 61-65 62-63 63-64 66-67 66-70 67-68 71-72 71-75 72-73 76-77 76-80 77-78 isolated ring systems: containing 1 : 16 : 51 : 56 : 61 : 66 : 71 : 76 : 88 : 93 : 98 : 103 : 108 : 113 : G1:0,N G2: [*1], [*2], [*3], [*4], [*5] G3: [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13], [*14], [*15], [*16], [*17] Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom 52:Atom 53:Atom 54:CLASS 55:Atom 56:Atom 57:Atom 58:Atom 59:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:CLASS 65:Atom 66:CLASS 67:CLASS 68:Atom 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:Atom 79:CLASS 80:CLASS 88:Atom 89:CLASS 90:CLASS 91:Atom 92:Atom 93:Atom 94:CLASS 95:CLASS 96:Atom 97:Atom 98:Atom 99:CLASS 100:CLASS 101:Atom 102:Atom 103:Atom 104:CLASS 105:CLASS 106:Atom 107:Atom 108:Atom 109:CLASS 110:CLASS 111:Atom 112:Atom 113:Atom 114:CLASS 115:CLASS 116:Atom 117:Atom 127:CLASS Generic attributes : 11: Saturation : Unsaturated 19: Saturation : Unsaturated 23: Saturation : Unsaturated 32: Saturation : Unsaturated 37: Saturation : Unsaturated Element Count : Node 47: Limited C, C1-5

L10 STRUCTURE UPLOADED

=> d 110 L10 HAS NO ANSWERS L10 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 110 sss sam SAMPLE SEARCH INITIATED 15:05:26 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 427 TO ITERATE

100.0% PROCESSED 427 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

7301 TO 9779

PROJECTED ANSWERS:

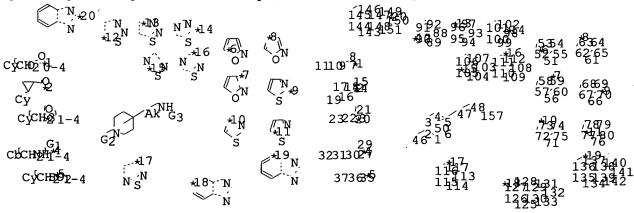
1 TO 80

L11

1 SEA SSS SAM L10

=> =>

Uploading C:\Program Files\Stnexp\Queries\10079452 (rce15).str



chain nodes :
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47
48 157
ring nodes :
1 2 3 4 5 6 16 17 18 51 52 53 54 55 56 57 58 59 60 61 62 63
64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 88 89 90 91
92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109
110 111 112 113 114 115 116 117 125 126 127 128 129 130 131 132 133
134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149
150 151

```
chain bonds :
2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30
 30-31 31-32 35-36 36-37 47-48 48-157
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 51-52 51-55 52-53 53-54
54-55 56-57 56-60 57-58 58-59 59-60 61-62 61-65 62-63 63-64 64-65 66-67
66-70 67-68 68-69 69-70
                            71-72 71-75 72-73 73-74 74-75 76-77
                                                                        76-80
78-79 79-80 88-89 88-92 89-90 90-91 91-92 93-94 93-97 94-95 95-96 96-97
98-99 98-102 99-100 100-101 101-102 103-104 103-107 104-105 105-106
106-107 108-109 108-112
                           109-110 110-111
                                              111-112
                                                       113-114
                                                                 113-117
                                                                          114-115
115-116 116-117 125-126
                           125-130
                                     126-127
                                              127-128
                                                       128-129
                                                                 129-130
                                                                          129-131
        131-132 132-133
130-133
                           134-135
                                     134-139
                                              135-136
                                                        136-137
                                                                 137-138
                  140-141 141-142
138-140
         139-142
                                     143-144 143-148
                                                       144-145
                                                                145-146
         147-149 148-151 149-150 150-151
147-148
exact/norm bonds :
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 10-11 14-15 16-19 20-21 22-23
27-29 27-30 36-37 47-48 48-157 54-55 59-60 64-65 68-69 69-70 73-74 74-75
 78-79 79-80 88-89 88-92 89-90 90-91 91-92 93-94 93-97 94-95 95-96 96-97
 98-99 98-102 99-100 100-101 101-102 103-104 103-107 104-105 105-106
106-107 108-109 108-112 109-110 110-111 111-112 113-114 113-117 114-115
115-116 116-117 129-130 129-131 130-133 131-132 132-133 138-139 138-140
139-142 140-141 141-142 147-148 147-149 148-151 149-150 150-151
exact bonds :
9-10 \quad 14-18 \quad 16-17 \quad 16-18 \quad 17-18 \quad 20-22 \quad 30-31 \quad 31-32 \quad 35-36 \quad 51-52 \quad 51-55 \quad 52-53
53-54 56-57 56-60 57-58 58-59 61-62 61-65 62-63 63-64 66-67 66-70 67-68
71-72 71-75 72-73 76-77 76-80 77-78 125-126 125-130 126-127 127-128
128-129 134-135 134-139 135-136 136-137 137-138 143-144 143-148 144-145
145-146 146-147
isolated ring systems:
containing 1 : 16 : 51 : 56 : 61 : 66 : 71 : 76 : 88 : 93 : 98 : 103 : 108 : 113 :
125 : 134 : 143 :
G1:0,N
G2: [*1], [*2], [*3], [*4], [*5]
G3:[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16],[*17],[*18],[*1
9],[*20]
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom 35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom
52:Atom 53:Atom 54:CLASS 55:Atom 56:Atom 57:Atom 58:Atom 59:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:CLASS 65:Atom 66:CLASS 67:CLASS 68:Atom 69:CLASS
 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:Atom 79:CLASS 80:CLASS 88:Atom 89:CLASS 90:CLASS 91:Atom 92:Atom 93:Atom
 94:CLASS 95:CLASS 96:Atom 97:Atom 98:Atom 99:CLASS 100:CLASS 101:Atom
102:Atom 103:Atom 104:CLASS 105:CLASS 106:Atom 107:Atom 108:Atom 109:CLASS
110:CLASS 111:Atom 112:Atom 113:Atom 114:CLASS 115:CLASS 116:Atom 117:Atom
125:Atom 126:Atom 127:Atom 128:Atom 129:Atom 130:Atom 131:Atom 132:Atom
133:Atom 134:Atom 135:Atom 136:Atom 137:Atom 138:Atom 139:Atom 140:Atom
141:Atom 142:Atom 143:Atom 144:Atom 145:Atom 146:Atom 147:Atom 148:Atom
149:Atom 150:Atom 151:Atom 157:CLASS
Generic attributes :
```

11:

10/079,452 (RCE)

Saturation : Unsaturated

19:

: Unsaturated Saturation

Saturation : Unsaturated

32:

: Unsaturated Saturation

37:

Saturation : Unsaturated

Element Count : Node 47: Limited C,C1-5

L12 STRUCTURE UPLOADED

=> d 112

L12 HAS NO ANSWERS

STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 112 sss sam

SAMPLE SEARCH INITIATED 15:09:08 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 428 TO ITERATE

100.0% PROCESSED 428 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

7319 TO 9801

PROJECTED ANSWERS:

1 TO 80

L13 1 SEA SSS SAM L12

=> s 112 sss ful

FULL SEARCH INITIATED 15:10:18 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 9020 TO ITERATE

100.0% PROCESSED 9020 ITERATIONS 21 ANSWERS

SEARCH TIME: 00.00.01

21 SEA SSS FUL L12

=> => s 114

8 L14 L15

=> d 115 1-8 bib, ab, hitstr

```
L15
    ANSWER 1 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
     2004:1080888 CAPLUS
AN
DN
     142:56340
     4-Heteroarylamino-substituted 3-fluoro-piperidines as NMDA/NR2B
TI
     antagonists, and their preparation, pharmaceutical compositions, and
     methods of use
IN
     Liverton, Nigel J.; Claiborne, Christopher F.; Claremon, David A.;
     McCauley, John A.
PA
     Merck & Co., Inc., USA
     PCT Int. Appl., 41 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
                               20041216
PΙ
     WO 2004108705
                          A1
                                            ∕WO 2004-US17175
                                                                   20040528
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CA, DE, DK, MM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, II, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
PRAI US 2003-475938P
                          P
                                20030604
     Title compds. I and their pharmaceutically acceptable salts are disclosed
     [wherein: HetAr is a 5- or 6-membered heteroarom. ring containing 1 or 2 N
     ring atoms, thiazolyl, or thiadiazolyl; HetAr is optionally substituted
     with 1 or 2 substituents, each substituent independently is C1-4 alkyl, F,
     Cl, Br, or iodo; A is a bond or Cl-2 alkylene; and B is
     aryl-(CH2)0-3OC(O)-, indanyl-(CH2)0-3OC(O)-, aryl-(CH2)1-3C(O)-,
     arylcyclopropyl-C(0)-, or aryl-(CH2)1-3NHC(0)-, wherein any aryl is
     optionally substituted by 1-5 substituents, each substituent is
     independently C1-4 alkyl, F, or C1]. I are effective as NMDA NR2B
     antagonists, useful for treating conditions such as, for example,
     Parkinson's disease, Alzheimer's disease, migraine, epilepsy and pain.
     Seven specific examples are claimed, and these plus various salts were
     prepared For instance, invention compound II was prepared in 8 steps: (1)
     coupling of CDI with 4-MeC6H4CH2OH and 4-piperidone HCl; (2)
     \alpha-fluorination of the piperidone carbonyl; (3) Witting reaction of
     the piperidone carbonyl with Ph3P:CHCO2Et; (4) stereoselective reduction of
     the resulting olefin to give primarily cis-isomeric ester III; (5) alkaline
     saponification of the Et ester; (6) conversion of the resulting acid to an
amine
     with diphenylphosphoryl azide; (7) heteroarylation of the amine with
     2-chloropyrimidine; and (8) chiral HPLC. In both (1) a cell-based
     functional assay to determine IC50 for inhibition of NR1A/NR2B receptors in
     Ltk- cells, and (2) a radioligand binding assay using tritiated AMD-2
     (preparation given) to determine Ki, compds. I had values of less than 50 μM,
     with these values advantageously being even lower than 0.1 μM.
IT
     808733-03-1P, (-)-cis-4-Methylbenzyl 3-fluoro-4-[(1,3,4-thiadiazol-
     2-ylamino)methyl]piperidine-1-carboxylate 808733-04-2P,
     (+)-trans-4-Methylbenzyl 3-fluoro-4-[(1,3,4-thiadiazol-2-
```

ylamino)methyl]piperidine-1-carboxylate 808733-11-1P,

(-)-cis-4-Methylbenzyl 3-fluoro-4-[(1,3,4-thiadiazol-2ylamino)methyl]piperidine-1-carboxylate hydrochloride
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(drug candidate; preparation of heteroarylamino-substituted fluoropiperidines as NMDA/NR2B receptor antagonists)

RN 808733-03-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Rotation (-). Absolute stereochemistry unknown.

RN 808733-04-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Rotation (+). Absolute stereochemistry unknown.

RN 808733-11-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Rotation (-). Absolute stereochemistry unknown.

● HCl

```
ANSWER 2 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
L15
AN
     2003:855758 CAPLUS
DN
     139:364829
ΤI
     Preparation of heterocyclo inhibitors of potassium channel function
IN
     Lloyd, John; Jeon, Yoon T.; Finlay, Heather; Yan, Lin; Beaudoin, Serge;
     Gross, Michael F.
     Bristol-Myers Squibb Company, USA; Icagen, Inc.
PA
SO
     PCT Int. Appl., 330 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LА
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
                         ____
                                            _____
PΙ
     WO 2003088908
                          A2
                                20031030
                                            WO 2003-US11807
                                                                    20030416
     WO 2003088908
                          А3
                                20040527
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2004110793
                          A1
                                20040610
                                          US 2003-417355
                                                                   20030416
PRAI US 2002-374279P
                          Ρ
                                20020419
os
    MARPAT 139:364829
AB
     The title compds. [I; m, p = 0-3 (provided that the sum of m and p is at
     least 2); Q = NR1, O, S, SO, SO2; R1 = H, C(:W)NR6R7, SO2NR6R7, OCONR6R7,
     etc.; R2 = heteroaryl, heteroarylalkyl, aryl, etc.; J = a bond, alkylene;
     R3 = R5, OR5, SO2R5, etc.; R5 = CN, heteroaryl, aryl, etc.; R6, R7 = H,
     alkyl, OH, etc.; W = (un) substituted NH, N(CO2H), N(CN), N(SO2H), CH(NO2);
     Rx = H, alkyl, hydroxyalkyl, aryl, etc.], useful as inhibitors of
     potassium channel function (especially inhibitors of the Kv1 subfamily of
     voltage gated K+ channels, especially inhibitors Kv1.5 which has been linked to
     the ultra-rapidly activating delayed rectifier K+ current IKur) in the
     prevention and treatment of arrhythmia and IKur-associated conditions, were
     prepared E.g., a multi-step synthesis of II [starting from
     bis(2-chloroethyl)amine], was given. Pharmaceutical composition comprising the
     compound I is claimed.
TΤ
     619286-41-8P 619288-83-4P 619288-85-6P
     619288-87-8P 619288-89-0P 619288-91-4P
     619289-09-7P 619289-15-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of substituted piperidines as inhibitors of potassium channel
        function)
     619286-41-8 CAPLUS
RN
CN
     4-Piperidinecarboxamide, 1-[3-(4-fluorophenyl)-1-oxopropyl]-4-phenyl-N-(4-
```

phenyl-2-thiazolyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ Ph & & & \\ & & \\ & & \\ & & \\ \end{array}$$

RN 619288-83-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-(3-isoxazolylamino)-2-oxoethyl]-4-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

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RN 619288-85-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-[(3-methyl-5-isoxazolyl)amino]-2-oxoethyl]-4-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 619288-87-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-[(5-methyl-3-isoxazolyl)amino]-2-oxoethyl]-4-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 619288-89-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-oxo-2-(2-thiazolylamino)ethyl]-4-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & | \\
 & C - O - CH_2 - Ph \\
\hline
 & S & Ph
\end{array}$$

RN 619288-91-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-oxo-2-(1,3,4-thiadiazol-2-ylamino)ethyl]-4-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 619289-09-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-oxo-2-[[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]amino]ethyl]-4-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
0 \\
\parallel \\
C-O-CH_2-Ph
\end{array}$$
F3C

RN 619289-15-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-oxo-2-[(4-phenyl-2-thiazolyl)amino]ethyl]-4-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & & O \\
Ph & & NH-C-CH_2-Ph \\
\hline
\end{array}$$

```
L15
    ANSWER 3 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
     2002:964146 CAPLUS
AN
DN
     138:39187
TI
     Preparation of piperidinecarboxylates and related compounds as NMDA NR2B
                                                           Common Arriques
     receptor antagonists for the treatment or prevention of migraine.
IN
     Allen, Christopher; Koblan, Ken S.; Sleeth, Timothy
PA
     Merck & Co., Inc., USA
SO
     PCT Int. Appl., 185 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
                         ____
                                                                  20020607
PΙ
     WO 2002100352
                          A2
                                20021219
                                            WO 2002-US21069
     WO 2002100352
                         Α3
                                20030327
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
             GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
             GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1399160
                          A2
                                20040324
                                            EP 2002-744807
                                                                   20020607
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                                                              No DP
     JP 2004537526
                          Т2
                                20041216
                                            JP 2003-503178
                                                                    20020607
     US 2004204341
                          A1
                                20041014
                                            US 2003-479923
                                                                   20031205
PRAI US 2001-297672P
                          Ρ
                                20010612
     WO 2002-US21069
                          W
                                20020607
     A method for treating or preventing migraines comprises administration of
     an NR2B receptor antagonist (no data). The invention also encompasses the
     combination of an NR2B antagonist with a cyclooxygenase-2 selective
     inhibitor, a calcitonin gene-related peptide receptor (CGRP) ligand, a
     leukotriene receptor antagonist, or a 5HT1B/1D agonist for the treatment
     or prevention of migraines. Thus, 4-hydroxybenzoic acid,
     1-hydroxybenzotriazole hydrate, benzyl 4-(aminomethyl)piperidine-1-
     carboxylate (preparation given), and Et3N in DMF were treated with
     1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride and the mixture
     allowed to stir at room temperature for 18 h to give 4-[(4-
     hydroxybenzoylamino)methyl]piperidine-1-carboxylic acid benzyl ester.
TΤ
     455265-21-1P, Benzyl 4-[(3-isoxazolylamino)methyl]-1-
     piperidinecarboxylate 455265-28-8P, Benzyl 4-[(1,3,4-thiadiazol-
     2-ylamino)methyl]-1-piperidinecarboxylate 455265-46-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of piperidinecarboxylates and related compds. as NR2B receptor
        antagonists for the treatment or prevention of migraine)
     455265-21-1 CAPLUS
RN
CN
     1-Piperidinecarboxylic acid, 4-[(3-isoxazolylamino)methyl]-, phenylmethyl
     ester (9CI) (CA INDEX NAME)
```

$$0 \\ C-O-CH_2-Ph$$

$$0 \\ NH-CH_2$$

RN 455265-28-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(1,3,4-thiadiazol-2-ylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$N = NH - CH_2 - Ph$$

RN 455265-46-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-thiazolylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O \\
C - O - CH_2 - Ph
\end{array}$$

$$\begin{array}{c|c}
N \\
C - O - CH_2 - Ph
\end{array}$$

```
L15
    ANSWER 4 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
AN
     2002:676010 CAPLUS
DN
     137:216875
ΤI
     Preparation of N-acyl-4-(heterocyclylaminomethyl)piperidines as NMDA/NR2B
IN
     Claiborne, Christopher F.; Butcher, John W.; Claremon, David A.; Libby,
     Brian E.; Liverton, Nigel J.; Munson, Peter M.; Nguyen, Kevin T.;
     Phillips, Brian; Thompson, Wayne; McCauley, John A.
PA
     Merck & Co., Inc., USA
                                                                   Appl Put
     PCT Int. Appl., 208 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
                                             ______
PΙ
     WO 2002068409
                          A1
                                 20020906
                                           WO 2002-US5226
                                                                     20020220
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE; SN, TD, TG
     CA 2438895
                                 20020906
                          AΑ
                                             CA 2002-2438895
                                                                     20020220
     US 2002165241
                          A1
                                 20021107
                                             US 2002-79452
                                                                     20020220
                                             EE 2003-403
     EE 200300403
                          Α
                                 20031215
                                                                     20020220
     EP 1379520
                          A1
                                 20040114
                                             EP 2002-721105
                                                                     20020220
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002007526
                          Α
                                 20040309
                                             BR 2002-7526
                                                                     20020220
     JP 2004524314
                          T2
                                 20040812
                                             JP 2002-567923
                                                                     20020220
     US 2004209889
                          A1
                                 20041021
                                             US 2003-470561
                                                                     20030729
     NO 2003003732
                          Α
                                 20031022
                                             NO 2003-3732
                                                                     20030822
                                 20010223
PRAI US 2001-271100P
                          Ρ
     WO 2002-US5226
                          W
                                 20020220
OS
     MARPAT 137:216875
     BQ1(X)ANHQ2 [Q1 = 5-7 membered N-containing nonarom. ring, azabicyclooctyl; Q2
AB
     = 5-6 membered (substituted) heteroaryl ring; A = alkylene; B =
     Ar(CH2)0-302C, Ar(CH2)0-3S02, etc.; Ar = (substituted) aryl, heteroaryl; X
     = H, OH, F, alkyl, alkoxy, NH2, O], were prepared Thus,
     1-[(benzyloxy)carbonyl]-4-piperidinecarboxylic acid, 4-aminopyridine, EDC,
     and HOAt were kept 4 h in DMF to give the amide, which was reduced with
     BH3. THF to give benzyl 4-[(4-pyridylamino)methyl]-1-piperidinecarboxylate.
     Title compds. showed IC50's of <50 µM for inhibition of NR1A/2B NMDA
     receptor activation.
IT
     455265-21-1P 455265-28-8P 455265-46-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (claimed compound; preparation of
N-acyl-4-(heterocyclylaminomethyl)piperidine
        s as NMDA/NR2B antagonists)
RN
     455265-21-1 CAPLUS
CN
     1-Piperidinecarboxylic acid, 4-[(3-isoxazolylamino)methyl]-, phenylmethyl
```

ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O \\
\parallel \\
C-O-CH_2-Ph\\
\end{array}$$

RN 455265-28-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(1,3,4-thiadiazol-2-ylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$N \longrightarrow NH-CH_2 \longrightarrow N \longrightarrow C-O-CH_2-Ph$$

RN 455265-46-0 CAPLUS

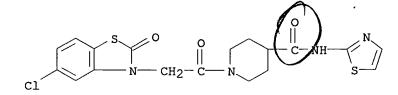
CN 1-Piperidinecarboxylic acid, 4-[(2-thiazolylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \circ \\
 & C - \circ - \circ CH_2 - Ph \\
\hline
 & \circ \\
 & C - \circ - \circ CH_2 - Ph \\
\hline
 & \circ \\
 & C - \circ - \circ CH_2 - Ph \\
\hline
 & \bullet \\
 &$$

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/079,452 (RCE)

- L15 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2002:251342 CAPLUS
- DN 137:262978
- TI Novel potent antagonists of human neuropeptide Y Y5 receptor. Part 1: 2-oxobenzothiazolin-3-acetic acid derivatives
- AU Tabuchi, Seiichiro; Itani, Hiromichi; Sakata, Yoshihiko; Oohashi, Hiroko; Satoh, Yoshinari
- CS Fujisawa Pharmaceutical Co., Ltd., Medicinal Chemistry Research Laboratories, Osaka, Yodogawa-ku, 532-851, Japan
- SO Bioorganic & Medicinal Chemistry Letters ((2002), 2(8), 1171-1175 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- OS CASREACT 137:262978
- AB Novel neuropeptide NPY-Y5 antagonist FR73966 I was discovered by screening of our inhouse chemical library. The analogs, e.g. II, were prepared by application of parallel synthesis techniques. Some of the resulting 2-oxobenzothiazolin-3-acetic acid derivs. exhibited nanomolar binding affinity for human NPY-Y5 receptors.
- IT 443686-48-4
 - RL: PAC (Pharmacological activity); BIOL (Biological study) (preparation of 2-oxobenzothiazolin-3-acetic acid derivs. as potent antagonists of human neuropeptide Y Y5 receptor)
- RN 443686-48-4 CAPLUS
- CN 4-Piperidinecarboxamide, 1-[(5-chloro-2-oxo-3(2H)-benzothiazolyl)acetyl]-N-2-thiazolyl- (9CI) (CA INDEX NAME)



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L15 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2002:136922 CAPLUS
- DN 137:103391
- TI Novel Potent Antagonists of Human Neuropeptide Y Y5 Receptors. Part 3: 7-Methoxy-1-hydroxy-1-substituted Tetraline Derivatives
- AU Itani, Hiromichi; Ito, Harunobu; Sakata, Yoshihiko; Hatakeyama, Yoshifumi; Oohashi, Hiroko; Satoh, Yoshinari
- CS Medicinal Chemistry Research Laboratories, Fujisawa Pharmaceutical Co., Ltd., Yodogawa-ku, Osaka, 532-8514, Japan
- SO Bioorganic & Medicinal Chemistry Letters (2002), 12(5), 799-802 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- OS CASREACT 137:103391
- As a part of our continuing research on NPY-Y5 receptor antagonists in the series of novel 6-methoxybenzo[a]cycloheptene derivs., we discovered a novel skeleton, 7-methoxy-1-hydroxytetraline which had been used as an intermediate, to be more suitable for increasing potencies leading to compound Addnl., we discovered that the naphthalenesulfonamide moiety which was thought to be an essential pharmacophore could be replaced by the 5-chlorobenzothiazolin-3-acetic acid moiety to lead to potent compound The structure-activity relationships on compds. and their related derivs. are described. Unfortunately, although compds. and had very high affinities for Y5 receptors, their poor permeabilities to brain were shown by exo-vivo binding assays when orally administered.

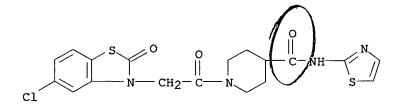
IT 443686-48-4

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(novel potent antagonists of human neuropeptide Y Y5 receptors from 7-methoxy-1-hydroxy-1-substituted tetraline derivs.)

RN 443686-48-4 CAPLUS

CN 4-Piperidinecarboxamide, 1-[(5-chloro-2-oxo-3(2H)-benzothiazolyl)acetyl]-N-2-thiazolyl- (9CI) (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:463221 CAPLUS

DN 135:61247

TI Preparation of sulfonylaminomethylpiperidinylethylamines for antiobesity, antidiabetics, and antihypertensives

IN Sato, Yoshinari; Itani, Hiromichi; Ito, Tatsunobu; Sakata, Yoshihiko; Hatakeyama, Yoshifumi; Ohashi, Hiroko

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 64 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
				AITBICATION NO.	DAIL
ΡI	JP 2001172257	A2	20010626	JP 2000-302567	20001002
PRAI	JP 1999-284407	Α	19991005		

OS MARPAT 135:61247

The compds. R1R2(NR6)pR5AR3(SO2)sR4 [R1 = (un)substituted (un)saturated C ring, heterocyclyl; R2 = bond, (un)substituted lower alkylene; R3 = piperidinediyl, (CH2)n, CHR7, NH, CO; R7 = indolylmethyl; n = 1-4; R4 = (un)substituted aryl, aralkyl, heterocyclyl; R5 = bond, lower alkylene, (CH2)mCO; m = 0-1; R6 = H, OH; A = N-containing saturated heterocyclylene; p = 0-1; s = 0-1] are prepared N-[[4-[(naphthalen-1-yl)sulfonylaminomethyl]piperidin-1-yl]carbonylmethyl]-2-indolinecarboxamide (263.0 mg) was reacted with borane-Me2S complex in THF under reflux for 2 h and treated with HCl under reflux for 1 h to give 104.8 mg N-(indolin-2-yl)methyl-N-[4-[(naphthalen-1-yl)sulfonylaminomethyl]piperidin-1-yl]ethylamine hydrochloride showing good inhibitory activity against neuropeptide Y receptor in vitro.

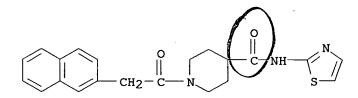
IT 345955-47-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of sulfonylaminomethylpiperidinylethylamines for antiobesity, antidiabetics, and antihypertensives)

RN 345955-47-7 CAPLUS

CN 4-Piperidinecarboxamide, 1-(2-naphthalenylacetyl)-N-2-thiazolyl- (9CI) (CA INDEX NAME)



- L15 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2001:372159 CAPLUS
- DN 134:366868
- TI Preparation of benzothiazolines as neuropeptide Y receptor antagonists
- IN Sato, Yoshiya; Itani, Hiromichi; Tabuchi, Seiichiro; Sakata, Yoshihiko; Ohashi, Hiroko
- PA Fujisawa Pharmaceutical Co., Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 88 pp. CODEN: JKXXAF
- DT Patent
- LA Japanese

FAN. CNT 1

22411	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PRAI	JP 2001139574 AU 1999-3093	A2 A	20010522 19990928	JP 2000-296175	20000928

- OS MARPAT 134:366868
- AB The title compds. I [R1 = H, halo; W = S, O; A = (CH2)n, etc.; n = 1 6; Z = (un)substituted N-containing heterocyclic ring] are prepared 1-[(5-Chloro-2-oxobenzothiazolin-3-yl)acetyl]piperidine-4-carboxylic acid 4-benzoylanilide showed IC100 of 10-7 M in a neuropeptide Y5 receptor binding assay.
- IT 340178-52-1P 340178-59-8P 340178-81-6P 340179-04-6P 340179-05-7P
 - RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
- (preparation of benzothiazolines as neuropeptide Y receptor antagonists) RN 340178-52-1 CAPLUS
- CN 4-Piperidinecarboxamide, 1-[(5-chloro-2-oxo-3(2H)-benzothiazolyl)acetyl]-N-(5-methyl-2-thiazolyl)- (9CI) (CA INDEX NAME)

- RN 340178-59-8 CAPLUS
- CN 4-Piperidinecarboxamide, 1-[(5-chloro-2-oxo-3(2H)-benzothiazolyl)acetyl]-N-[5-(1,1-dimethylethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)

- RN 340178-81-6 CAPLUS
- CN 4-Piperidinecarboxamide, N-(5-acetyl-4-methyl-2-thiazolyl)-1-[(5-chloro-2-oxo-3(2H)-benzothiazolyl)acetyl]- (9CI) (CA INDEX NAME)

RN 340179-04-6 CAPLUS

CN 4-Piperidinecarboxamide, 1-[(2-oxo-3(2H)-benzoxazolyl)acetyl]-N-2-thiazolyl- (9CI) (CA INDEX NAME)

RN 340179-05-7 CAPLUS

CN 4-Piperidinecarboxamide, 1-[(2-oxo-3(2H)-benzothiazolyl)acetyl]-N-2-thiazolyl- (9CI) (CA INDEX NAME)

10/079,452 (RCE)

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(FILE 'HOME' ENTERED AT 14:51:54 ON 21 JAN 2005)

	FILE 'REGISTRY' ENTERED AT 14:51:59 ON 21 JAN 2005
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L2	SCREEN 2016 OR 2039 OR 2040 OR 2045 OR 2047
L3	STRUCTURE UPLOADED
L4	QUE L3 AND L1 NOT L2
L5	0 S L4 SSS SAM
L6	STRUCTURE UPLOADED
L7	1 S L6 SSS SAM
L8	STRUCTURE UPLOADED
L9	O S L8 SSS SAM
L10	STRUCTURE UPLOADED
L11	1 S L10 SSS SAM
L12	STRUCTURE UPLOADED
L13	1 S L12 SSS SAM
L14	21 S L12 SSS FUL
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L15 8 S L14

FILE 'CAOLD' ENTERED AT 15:11:51 ON 21 JAN 2005

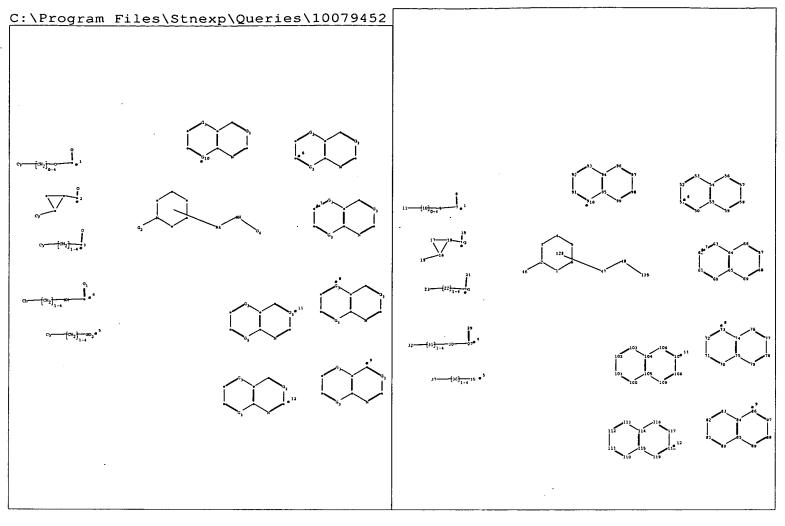
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L16 0 L14

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FULL ESTIMATED COST	ENTRY 0.43	SESSION 215.29
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY 0.00	SESSION -5.84

STN INTERNATIONAL LOGOFF AT 15:12:04 ON 21 JAN 2005



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chain nodes :
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                              19
                                   20
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                                               23
                                                    27
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                                                            30
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                                                                         35
                                                                             36
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       47
    46
            48
                 135
ring nodes :
          3
                 5
                       16 17 18 50 51 52 53 54 55 56
                                                                 57
             4
                    6
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                                                                          59
                                                                             60
                    65 66 67 68 69 70 71 72 73 74 75 76
        62
            63
                 64
                                                                       77 78 79
                             86 87 88 89
            82
                83
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        100 101 102
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                                 105 106
                                            107
                                                  108 109 110
                                                                  111
    114
         115
             116 117
                         118
                              119
chain bonds :
               7-9 9-10 10-11
    2-46 7-8
                                 14-15 14-18 16-19 20-21
                                                                20-22
                                                                        22-23
    27-29
           27-30 30-31 31-32
                                 35-36 36-37 47-48
                                                       48-135
ring bonds :
    1-2 1-6
              2-3
                    3 - 4
                         4-5
                              5-6
                                   16-17
                                           16-18
                                                  17-18
                                                          50-51
                                                                 50-55
                                                                         51-52
    52-53
           53-54
                   54-55
                          54-56
                                 55-59
                                         56-57
                                                57-58
                                                        58-59
                                                               60-61
                                                                       60-65
                                                                              61-62
                                                        68-69
                                                                              71-72
    62-63
           63-64
                   64 - 65
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                                  65-69
                                         66-67
                                                67-68
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                   74-75
                          74-76
    72 - 73
           73 - 74
                                  75-79
                                         76-77
                                                77-78
                                                        78-79
                                                               80-81
                                                                       80-85
                                                                              81-82
                                                                       90-95 91-92
    82 - 83
                                 85-89
                                                87-88
           83-84
                   84-85
                          84-86
                                         86-87
                                                        88-89
                                                               90-91
    92-93
                          94-96
                                 95-99
                                         96-97
                                                97-98
                                                        98-99
           93 - 94
                   94 - 95
                                                                       100-105
                                                               100-101
                                104-105
    101-102
             102-103
                       103-104
                                          104-106
                                                   105-109 106-107
                                                                       107-108
    108-109
             110-111
                       110-115
                                111-112
                                          112-113
                                                   113-114
                                                             114-115
                                                                       114-116
    115-119
             116-117
                       117-118
                                118-119
exact/norm bonds :
                                    5-6
    1-2 1-6
              2-3
                   2-46
                          3-4 4-5
                                          7-8
                                               7-9 9-10 10-11
                                                                  14-15
                                                                          14-18
                          17-18
    16-17
           16 - 18
                   16-19
                                 20-21
                                         20-22
                                                                       30-31
                                                22-23
                                                               27-30
                                                        27-29
                                                                              31 - 32
    35-36
           36-37
                   47 - 48
                          48-135
                                  50-51
                                          50-55
                                                        52-53
                                                 51-52
                                                               53-54
                                                                       54-55
    54-56
           55-59
                   56-57
                          57-58
                                 58-59
                                         60-61
                                                60-65
                                                        61-62
                                                               62-63
                                                                       63-64
                                                                              64-65
    64-66
           65-69
                   66-67
                          67-68
                                  68-69
                                         70-71
                                                70-75
                                                        71-72
                                                               72-73
                                                                       73-74
                                                                              74-75
    74-76
           75-79
                   76-77
                          77~78
                                 78-79
                                         80-81
                                                80-85
                                                        81-82
                                                               82-83
                                                                       83-84
                                                                              84 - 85
    84-86
           85-89
                   86-87
                          87-88
                                 88-89
                                         90-91
                                                90-95
                                                        91-92
                                                               92-93
                                                                       93-94
                                                                              94 - 95
                                                           101-102
    94-96
           95-99
                   96-97
                          97~98
                                 98-99
                                         100-101
                                                  100-105
                                                                      102-103
    103-104
             104-105
                      104-106
                                105-109
                                          106-107
                                                   107-108
                                                             108-109
                                                                       110-111
    110-115
             111-112
                       112-113
                                113-114
                                          114-115
                                                   114-116
                                                             115-119
                                                                       116-117
    117-118
             118-119
isolated ring systems :
```

```
G1:0, N
G2: [*1], [*2], [*3], [*4], [*5]
G3:C,N
G4: [*6], [*7], [*8], [*9], [*10], [*11], [*12]
Match level :
            2:Atom
                    3:Atom 4:Atom 5:Atom 6:Atom
                                                     7:CLASS
                                                              8:CLASS
                                                                       9:CLASS
    1:Atom
                                 15:CLASS
    10:CLASS
              11:Atom 14:CLASS
                                           16:Atom
                                                     17:Atom
                                                              18:Atom
                                                                      19:Atom
    20:CLASS
              21:CLASS
                        22:CLASS
                                 23:Atom
                                           27:CLASS
                                                     29:CLASS
                                                                30:CLASS
    31:CLASS
              32:Atom
                       35:CLASS
                                 36:CLASS
                                          .37:Atom
                                                     46:CLASS
                                                               47:CLASS
                                                     54:Atom 55:CLASS
    48:CLASS
              50:CLASS
                        51:Atom
                                 52:Atom
                                          53:CLASS
                                                                        56:CLASS
    57:CLASS
              58:CLASS
                                                              63:CLASS
                        59:Atom
                                 60:CLASS
                                            61:Atom
                                                     62:Atom
                                                                        64:Atom
                                                                71:Atom
    65:CLASS
              66:CLASS
                       67:CLASS
                                  68:CLASS
                                           69:Atom
                                                     70:CLASS
                                                                         72:Atom
                       75:CLASS
                                 76:CLASS
    73:CLASS
                                           77:CLASS
                                                      78:CLASS
                                                                79:Atom
              74:Atom
    80:CLASS
                       82:Atom 83:CLASS
                                          84:Atom 85:CLASS
                                                              86:CLASS 87:CLASS
              81:Atom
    88:CLASS
              89:Atom
                       90:CLASS
                                 91:Atom 92:Atom 93:CLASS
                                                              94:Atom 95:CLASS
    96:CLASS
              97:CLASS
                        98:CLASS
                                  99:Atom 100:CLASS
                                                      101:Atom 102:Atom
    103:CLASS
               104:Atom
                         105:CLASS
                                   106:CLASS
                                               107:CLASS 108:CLASS 109:Atom
    110:CLASS
               111:Atom
                         112:Atom 113:CLASS
                                              114:Atom 115:CLASS
                                                                   116:CLASS
    117:CLASS
               118:CLASS
                          119:Atom
                                   128:CLASS
                                              135:CLASS
Generic attributes :
    11:
    Saturation
                           : Unsaturated
    19:
    Saturation
                           : Unsaturated
    23:
    Saturation
                           : Unsaturated
    32:
    Saturation
                           : Unsaturated
    37:
    Saturation
                           : Unsaturated
```

containing 1 : 16 : 50 : 60 : 70 : 80 : 90 : 100 : 110 :

Element Count :

Node 47: Limited C,C1-5

=>
Uploading C:\Program Files\Stnexp\Queries\10079452 (rce19).str

chain nodes : 7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47 48 56 63 68 ring nodes : 1 2 3 4 5 6 16 17 18 50 51 52 53 54 55 57 58. 59 60 61 62 69 chain bonds : 2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30 30-31 31-32 35-36 36-37 47-48 47-68 48-69 51-56 58-63 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 50-51 50-55 51-52 52-53 53-54 54-55 57-58 57-62 58-59 59-60 60-61 61-62 exact/norm bonds : $1-2 \quad 1-6 \quad 2-3 \quad 2-46 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-9 \quad 10-11 \quad 14-15 \quad 16-19 \quad 20-21 \quad 22-23$ 27-29 27-30 36-37 47-48 47-68 48-69 50-51 50-55 51-52 51-56 52-53 53-54 54-55 57-58 57-62 58-59 58-63 59-60 60-61 61-62 Page 1

10/079,452 (RCE) exact bonds : 9-10 14-18 16-17 16-18 17-18 20-22 30-31 31-32 35-36 isolated ring systems : containing 1 : 16 : 50 : 57 : G1:0,N G2:[*1],[*2],[*3],[*4],[*5] G3: [*6], [*7], [*8] Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom 35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 68:CLASS 69:CLASS Generic attributes : 11: Saturation : Unsaturated 19: Saturation : Unsaturated 23: Saturation : Unsaturated 32: : Unsaturated Saturation 37: : Unsaturated Saturation

Element Count : Node 47: Limited C,C1-5

L1STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam SAMPLE SEARCH INITIATED 15:32:10 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 233718 TO ITERATE

1000 ITERATIONS 0.4% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE** BATCH **INCOMPLETE** PROJECTED ITERATIONS: EXCEEDS 1000000 PROJECTED ANSWERS: **EXCEEDS** L2 0 SEA SSS SAM L1 Uploading C:\Program Files\Stnexp\Queries\10079452 (rce20).str Cy CH 200-4 11⁻10⁻9⁻⁻74 1771824 I G3 ا 68 29 32⁻31⁻30⁻2⁴ 37⁻³⁶-35⁵

chain nodes :
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47
48 56 63 68
ring nodes :
1 2 3 4 5 6 16 17 18 50 51 52 53 54 55 57 58 59 60 61 62 70
71 72 73

10/079,452 (RCE)

chain bonds:
2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30 30-31 31-32 35-36 36-37 47-48 47-68 48-70 51-56 58-63 ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 50-51 50-55 51-52 52-53 53-54 54-55 57-58 57-62 58-59 59-60 60-61 61-62 70-71 70-73 71-72 72-73 exact/norm bonds:
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 9-10 10-11 14-15 14-18 16-17 16-18 16-19 17-18 20-21 20-22 22-23 27-29 27-30 30-31 31-32 35-36 36-37 47-48 47-68 48-70 50-51 50-55 51-52 51-56 52-53 53-54 54-55 57-58 57-62 58-59 58-63 59-60 60-61 61-62 70-71 70-73 71-72 72-73 isolated ring systems: containing 1: 16: 50: 57:

G1:0,N

G2: [*1], [*2], [*3], [*4], [*5]

G3: [*6], [*7], [*8]

G4:C,N

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom 35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 68:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS Generic attributes:

11:

Saturation : Unsaturated

19:

Saturation : Unsaturated

23:

Saturation : Unsaturated

32:

Saturation : Unsaturated

37:

Saturation : Unsaturated

Element Count : Node 47: Limited C,C1-5

L3 STRUCTURE UPLOADED

=> d 13 L3 HAS NO ANSWERS L3 STR

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

 \Rightarrow s 13 sss sam

SAMPLE SEARCH INITIATED 15:35:04 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 233718 TO ITERATE

1000 ITERATIONS 0.4% PROCESSED

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

EXCEEDS 1000000

PROJECTED ANSWERS:

EXCEEDS 0

L4

0 SEA SSS SAM L3

=>

Uploading C:\Program Files\Stnexp\Queries\10079452 (rce21).str

```
chain nodes :
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47
48 135
ring nodes :
1 2 3 4 5 6 16 17 18 50 51 52 53 54 55 56 57 58 59 60 61 62
63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83
84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103
104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119
chain bonds :
2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30
30-31 31-32 35-36 36-37 47-48 48-135
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 50-51 50-55 51-52 52-53
53-54 54-55 54-56 55-59 56-57 57-58 58-59 60-61 60-65 61-62 62-63 63-64
64-65 64-66 65-69 66-67 67-68 68-69 70-71 70-75 71-72 72-73 73-74 74-75
74-76 75-79 76-77 77-78 78-79 80-81 80-85 81-82 82-83 83-84 84-85 84-86
85-89 86-87 87-88 88-89 90-91 90-95 91-92 92-93 93-94 94-95 94-96 95-99 96-97 97-98 98-99 100-101 100-105 101-102 102-103 103-104 104-105 104-106
```

```
exact/norm bonds :
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 9-10 10-11 14-15 14-18 16-17
16-18 16-19 17-18 20-21 20-22 22-23 27-29 27-30 30-31 31-32
                                                                 35-36
47-48 48-135 50-51 50-55 51-52
                                52-53 53-54
                                             54-55
                                                     54-56 55-59
                                                                 56-57
 58-59 60-61 60-65
                    61-62
                          62-63
                                 63-64
                                        64-65
                                              64-66
                                                    65-69
                                                           66-67
                                                                  67-68
70-71
      70-75
             71-72
                    72-73
                          73-74
                                 74-75
                                       74-76
                                              75-79
                                                     76-77
                                                           77-78
                                                                  78-79
                                              86-87
80-85 81-82 82-83
                    83-84 84-85
                                84-86
                                       85-89
                                                     87-88
                                                           88-89
                                                                  90-91
                                                                         90 - 95
91-92 92-93 93-94 94-95 94-96
                                 95-99 96-97 97-98 98-99 100-101
                                                                    100-105
101-102 102-103
                103-104 104-105
                                 104-106 105-109 106-107 107-108 108-109
       110-115
                111-112 112-113 113-114 114-115 114-116 115-119
110-111
                                                                  116-117
117-118 118-119
isolated ring systems :
containing 1 : 16 : 50 : 60 : 70 : 80 : 90 : 100 : 110 :
G1:0,N
G2:[*1],[*2],[*3],[*4],[*5]
G3:C,N
G4:[*6],[*7],[*8],[*9],[*10],[*11],[*12]
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 14:CLASS 15:CLASS
                           16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS
                 23:Atom 27:CLASS
                                   29:CLASS
                                             30:CLASS
                                                      31:CLASS
35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom
52:Atom 53:CLASS 54:Atom 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:Atom
60:CLASS 61:Atom 62:Atom 63:CLASS 64:Atom 65:CLASS 66:CLASS 67:CLASS
68:CLASS 69:Atom 70:CLASS 71:Atom 72:Atom 73:CLASS 74:Atom 75:CLASS
76:CLASS 77:CLASS 78:CLASS 79:Atom 80:CLASS 81:Atom 82:Atom 83:CLASS
84:Atom 85:CLASS 86:CLASS 87:CLASS 88:CLASS 89:Atom 90:CLASS 91:Atom
92:Atom 93:CLASS 94:Atom 95:CLASS 96:CLASS 97:CLASS 98:CLASS 99:Atom
100:CLASS 101:Atom 102:Atom 103:CLASS 104:Atom 105:CLASS 106:CLASS 107:CLASS
108:CLASS 109:Atom 110:CLASS 111:Atom 112:Atom 113:CLASS 114:Atom 115:CLASS
116:CLASS 117:CLASS 118:CLASS 119:Atom 128:CLASS 135:CLASS
Generic attributes:
11:
Saturation
                    : Unsaturated
19:
Saturation
                     : Unsaturated
23:
Saturation
                     : Unsaturated
32:
Saturation
                    : Unsaturated
37:
Saturation
                    : Unsaturated
```

Element Count : Node 47: Limited C,C1-5

C, C1-3

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 15 sss sam

SAMPLE SEARCH INITIATED 15:43:29 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 19631 TO ITERATE

5.1% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 384235 TO 401005

PROJECTED ANSWERS:

0 TO 0 0 ANSWERS

0 SEA SSS SAM L5 L6

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1840

L7 SCREEN CREATED

=> screen 2016 OR 2039 OR 2040 OR 2045 OR 2047

SCREEN CREATED Г8

=>

Uploading C:\Program Files\Stnexp\Queries\10079452 (rce22).str

```
chain nodes :
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47
48 135
ring nodes :
1 2 3 4 5 6 16 17 18 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103
104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119
chain bonds :
2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30
 30-31 31-32 35-36 36-37 47-48 48-135
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 50-51 50-55 51-52 52-53
53-54 54-55 54-56 55-59 56-57 57-58 58-59 60-61 60-65 61-62 62-63 63-64
64-65 64-66 65-69 66-67 67-68 68-69 70-71 70-75 71-72 72-73 73-74 74-75
74-76 75-79 76-77 77-78 78-79 80-81 80-85 81-82 82-83 83-84 84-85 84-86
85-89 86-87 87-88 88-89 90-91 90-95 91-92 92-93 93-94 94-95 94-96 95-99
96-97 97-98 98-99 100-101 100-105 101-102 102-103 103-104 104-105 104-106
105-109 106-107 107-108 108-109 110plot 9110-115 111-112 112-113 113-114 114-115 114-116 115-119 116-117 117-118 118-119
```

```
exact/norm bonds :
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 9-10 10-11 14-15 14-18 16-17
16-18 16-19 17-18 20-21 20-22 22-23 27-29 27-30 30-31 31-32
47-48 48-135 50-51 50-55 51-52 52-53 53-54 54-55
                                                    54-56 55-59 56-57
 58-59 60-61 60-65
                    61-62
                         62-63 63-64
                                       64-65 64-66
                                                    65-69
                                                           66-67
                                                                  67-68 68-69
 70-71 70-75
             71-72
                    72-73
                          73-74
                                74-75
                                       74-76
                                             75-79
                                                     76-77
                                                           77-78
                                                                  78-79
 80-85 81-82 82-83
                    83-84
                          84-85
                                84-86
                                       85-89
                                              86-87
                                                     87-88
                                                           88-89
                                                                  90-91
91-92 92-93 93-94 94-95 94-96
                                95-99 96-97 97-98 98-99 100-101 100-105
101-102 102-103 103-104 104-105 104-106 105-109 106-107 107-108 108-109
       110-115
                111-112 112-113 113-114 114-115 114-116 115-119
110-111
                                                                  116-117
117-118 118-119
isolated ring systems :
containing 1 : 16 : 50 : 60 : 70 : 80 : 90 : 100 : 110 :
G1:0,N
G2: [*1], [*2], [*3], [*4], [*5]
G3:C,N
G4:[*6],[*7],[*8],[*9],[*10],[*11],[*12]
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS
                 23:Atom 27:CLASS 29:CLASS 30:CLASS
                                                      31:CLASS
35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom
52:Atom 53:CLASS 54:Atom 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:Atom
60:CLASS 61:Atom 62:Atom 63:CLASS 64:Atom 65:CLASS 66:CLASS 67:CLASS
68:CLASS 69:Atom 70:CLASS 71:Atom 72:Atom 73:CLASS 74:Atom 75:CLASS
76:CLASS 77:CLASS 78:CLASS 79:Atom 80:CLASS 81:Atom 82:Atom 83:CLASS
84:Atom 85:CLASS 86:CLASS 87:CLASS 88:CLASS 89:Atom 90:CLASS 91:Atom
92:Atom 93:CLASS 94:Atom 95:CLASS 96:CLASS 97:CLASS 98:CLASS 99:Atom
100:CLASS 101:Atom 102:Atom 103:CLASS 104:Atom 105:CLASS 106:CLASS 107:CLASS
 108:CLASS 109:Atom 110:CLASS 111:Atom 112:Atom 113:CLASS 114:Atom 115:CLASS
116:CLASS 117:CLASS 118:CLASS 119:Atom 128:CLASS 135:CLASS
Generic attributes :
11:
Saturation
                    : Unsaturated
19:
Saturation
                    : Unsaturated
23:
Saturation
                    : Unsaturated
32:
Saturation
                    : Unsaturated
37:
Saturation
                    : Unsaturated
```

Element Count : Node 47: Limited C,C1-5

L9 STRUCTURE UPLOADED

=> que L9 AND L7 NOT L8

L10 QUE L9 AND L7 NOT L8

=> d 110

L8

L10 HAS NO ANSWERS

L7

SCR 2016 OR 2039 OR 2040 OR 2045 OR 2047

L9 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

SCR 1840

Structure attributes must be viewed using STN Express query preparation. QUE L9 AND L7 NOT L8 L10

=> s 110 sss sam

SAMPLE SEARCH INITIATED 15:44:47 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 18683 TO ITERATE

5.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

365479 TO 381841

PROJECTED ANSWERS:

0 TO Ω

L11 O SEA SSS SAM L9 AND L7 NOT L8

=> s 110 sss ful

FULL SEARCH INITIATED 15:44:56 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 371334 TO ITERATE

100.0% PROCESSED 371334 ITERATIONS SEARCH TIME: 00.00.07

11 ANSWERS

11 SEA SSS FUL L9 AND L7 NOT L8

=> => s 112

7 L12 L13

=> d 113 1-7 bib, ab, hitstr

- L13 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2004:963181 CAPLUS
- DN 141:379941
- TI Preparation of quinazoline-2,4-diamines as melanin concentrating hormone (MCH) receptor antagonists
- IN Sekiguchi, Yoshikatsu; Kanuma, Yukihiro; Omodera, Katsunori; Tran, Thuy-ahn; Kramer, Bryan Aubrey; Beeley, Nigel Robert Arnold
- PA Taisho Pharmaceutical Co., Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 988 pp. CODEN: JKXXAF
- DT Patent
- LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE
PI JP 2004315511 A2 (20041111 JP 2004-95046 20040329
PRAI JP 2003-93418 A (20030331

AB The title compds. Q-L-Y-Rl [Q = Q1, H2NC(:NH); wherein R2 = NHNH2, NHNHBoc, (un)substituted NH2, morpholino, 4-acetyl-piperazinyl, 4-phenylpiperazinyl; R1 = each (un)substituted C1-16 alkyl, C2-8 alkenyl, C2-4 alkynyl, C3-6 cycloalkyl, C3-6 cycloalkenyl, carbocyclyl, carbocyclic alkyl, or heterocyclyl; L = each Q2-Q6 or its cis- or trans-isomer, Q7-Q16; R4 = H, C1-3 alkyl; R5 = H, each (un)substituted carbocyclic aryl or C1-3 alkyl; Y = SO2, CO, a single bond, CH2] or salts thereof are prepared These compds. are MCH receptor antagonists and used for regulating orphan G protein-coupled receptor SLC-1 and for the prevention and/or treatment of obesity, obesity-related diseases, anxiety, or depression. Thus, hydrogenolysis of benzyl cis-[[4-(4-dimethylaminoquinazolin-2-ylamino)cyclohexyl]methyl]carbamate over 5% Pd-C in MeOH at 50° under H atmospheric for 3 days gave a solution of

cis-[[4-(4-dimethylaminoquinazolin-

2-ylamino)cyclohexyl]methyl]amine in MeOH which underwent reductive alkylation with 4-bromo-2-trifluoromethoxybenzaldehyde and NaBH(OAc)3 in AcOH/CH2Cl2 to give, after purification using HPLC and treatment with 4 N HCl/EtOAc, compound (I).2HCl. In a high throughput function screen for identifying lead compds., I.2HCl inhibited the human MCH-induced cellular Ca2+ flux with IC50 of 6 μg/mL.

IT 510733-93-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

 $\hbox{ (preparation of quinazoline derivs. as melanin-concentrating hormone (MCH) }\\$

antagonists for prevention and/or treatment of obesity, obesity-related diseases, anxiety, or depression)

RN 510733-93-4 CAPLUS

CN 4-Piperidinemethanamine, 1-[[4-bromo-2-(trifluoromethoxy)phenyl]acetyl]-N[4-(dimethylamino)-2-quinazolinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
N & \text{NH} - \text{CH}_2 \\
\hline
N & \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c|c}
N & \text{O} & \text{C} - \text{CH}_2 \\
\hline
O - \text{CF}_3
\end{array}$$

$$\begin{array}{c|c}
N & \text{O} & \text{C} - \text{CH}_2 \\
\hline
O - \text{CF}_3
\end{array}$$

● HCl

Page 13

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L13
    ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AN
     2003:282325 CAPLUS
DN
     138:321285
TI
     Preparation of quinazoline-2,4-diamines as MCH receptor antagonists
     Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera, Katsunori; Tran, Thuy-anh;
IN
     Kramer, Bryan Aubrey; Beeley, Nigel Robert Arnold
PA
     Taisho Pharmaceutical Co., Ltd., Japan
SO
     PCT Int. Appl., 1171 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                                DATE
     PATENT NO.
                         KIND
                                            APPLICATION NO.
                                                                   DATE
                                            ----
                                                                   -----
PI
     WO 2003028641
                          A2
                                20030410
                                            WO 2002-US31059
                                                                   20020930
     WO 2003028641
                          A3
                                20030828
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1432693
                                20040630 EP 2002-800388
                         A2
                                                                   20020930
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
PRAI US 2001-326463P
                         Ρ
                                20011001
     US 2001-326758P
                          Ρ
                                20011002
     WO 2002-US31059
                          W
                                20020930
     MARPAT 138:321285
OS
AB
     The title compds. QLYR1[Q = I, C(:NH)NH2; R1 = (un)substituted alkyl,
     alkenyl, cycloalkyl, etc.; L = II-IV (wherein R4 = H, alkyl; R5 = H,
     alkyl, alkyl substituted by a substituted carbocyclic aryl), etc.; Y =
     SO2, CO, (CH2)m; m = 0-1] which act as MCH receptor antagonists, and are
     useful for prophylaxis or treatment of obesity, obesity related disorders,
     anxiety, or depression, were prepared Thus, hydrogenation of benzyl
     cis-[4-(4-dimethylaminoquinazolin-2-ylamino)cyclohexylmethyl]carbamate
     followed by reacting the resulting intermediate with 4-bromo-2-
     trifluoromethoxybenzaldehyde in the presence of NaBH(OAc)3 and AcOH in
     CH2Cl2, and treatment of the product with 4N HCl in EtOAc afforded 34%
     cis-V.2HCl which showed IC50 of 6 nM against MCH receptor.
IT
     510733-93-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of quinazoline-2,4-diamines as MCH receptor antagonists)
RN
     510733-93-4 CAPLUS
CN
     4-Piperidinemethanamine, 1-[[4-bromo-2-(trifluoromethoxy)phenyl]acetyl]-N-
     [4-(dimethylamino)-2-quinazolinyl]-, monohydrochloride (9CI) (CA INDEX
```

NAME)

HCl

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L13
    ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
     2003:97394 CAPLUS
AN
DN
     138:153541
TI
     Preparation of N-(1,5-naphthyridin-4-yl)piperidine-4-carboxamide
     derivatives as antibacterial agents
     Davies, David Thomas; Jones, Graham Elgin; Markwell, Roger Edward;
IN
     Pearson, Neil David
PA
     Smithkline Beecham PLC, UK
SO
     PCT Int. Appl., 97 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                                                                   DATE
                         KIND
                                DATE
                                            APPLICATION NO.
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                                ----<del>-</del>-
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    WO 2003010138
PΙ
                         A2
                                20030206
                                            WO 2002-EP8319
                                                                   20020725
     WO 2003010138
                         А3
                                20031204
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1419155
                                20040519
                                           EP 2002-764786
                         A2
                                                                   20020725
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     US 2004198756
                         A1
                                20041007
                                           US 2004-484563
                                                                   20040524
PRAI GB 2001-18238
                          Α
                                20010726
     WO 2002-EP8319
                          W
                                20020725
OS
     MARPAT 138:153541
     The title piperidine derivs. [I; one of Z1-Z5 is N, one is CR1a and the
AΒ
     remainder are CH, or one or two of Z1-Z5 are independently CR1 a and the
     remainder are CH; Rl, Rla = H, HO, Cl-6 alkoxy optionally substituted by
     (un) substituted C1-6 alkoxy, amino, piperidyl, guanidino or amidino, C1-6
     alkoxy-C1-6 alkyl, halo, C1-6 alkyl, C1-6 alkylthio, CF3, CF3O, etc.; R3 =
     CO2H, C1-6 alkoxycarbonyl, (un) substituted CONH2, cyano, tetrazolyl,
     (un) substituted 2-oxooxazolidinyl, 3-hydroxy-3-cyclobutene-1,2-dione-4-yl,
     2,4-thiazolidinedione-5-yl, tetrazol-5-ylaminocarbonyl, (un)substituted
     1,2,4-triazol-5-yl, 5-oxo-1,2,4-oxadiazol-3-yl, (un)substituted C1-4 alkyl
     or ethenyl, halogen, C1-6 alkylthio, CF3, C1-6 alkoxycarbonyl, C1-6
     alkylcarbonyl, C2-6 alkenyloxycarbonyl, C2-6 alkenylcarbonyl,
     (un) substituted OH or NH2, etc.; R31 is in the 2- or 3-position and is
     hydrogen or a group listed above for R3, provided that R31 in the
     2-position is not optionally substituted hydroxy, amino, trifluoromethyl
     or halogen; R4 = CH2R51, U-V-R52 (wherein R51 = C4-8 alkyl, hydroxy-C4-8
     alkyl, C1-4 alkoxy-C4-8 alkyl, etc.; U = CO, SO2, CH2 and V =
     (un) substituted CH2; or U = CH2 and V = CO, (un) substituted C(:NOH), SO2;
     R52 = (un) substituted bicyclic carbocyclic or heterocyclic ring); n = 0,1;
     AB = (un)substituted NHCO, CONH, COCH2, CH2CO, OCH2, CH2O, NHCH2, CH2NH,
     NHSO2, CH2 SO2, CH2CH2] and pharmaceutically acceptable derivs. thereof
     are prepared These compds. are useful in methods of treatment of bacterial
     infections in mammals, particularly man. Thus, 0.10 g
     4-(6-methoxy-[1,5]naphthyridin-4-ylcarbamoyl)-4-methylpiperidine and 0.095
     g 2-(3-0xo-3,4-dihydro-2H-benzo[1,4]thiazin-6-yl)ethyl methanesulfonate
```

were stirred with 138 mg K2CO3 in 2 mL DMF at room temperature for 3 days to give 4-methyl-1-[2-(3-oxo-3,4-dihydro-2H-benzo[1,4]thiazin-6-yl)ethyl]piperidine-4-carboxylic acid (6-methoxy-[1,5]naphthyridin-4-yl)amide (II). II oxalate showed min. inhibitory concentration of \leq 4 µg/mL against Staphylococcus aureus Oxford, S. aureus WCUH29, S. pneumoniae 1629, S. pneumoniae N1387, S. pneumoniae ERY 2, Enterococcus faecalis I, E. faecalis 7, Haemophilus influenzae Q1, H. influenzae NEMC1, Moraxella catarrhalis 1502, and Escherichia coli 7623.

IT 495414-76-1P 495414-90-9P 495414-91-0P,

4-Hydroxymethyl-4-(6-methoxy-[1,5]naphthyridin-4-ylcarbamoyl)piperidine-1-carboxylic acid benzyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of N-(1,5-naphthyridin-4-yl) piperidine-4-carboxamide derivs. as antibacterial agents)

RN 495414-76-1 CAPLUS

CN 1,4-Piperidinedicarboxylic acid, 4-[[(6-methoxy-1,5-naphthyridin-4-yl)amino]carbonyl]-, 4-(1,1-dimethylethyl) 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)

RN 495414-90-9 CAPLUS

CN 1,4-Piperidinedicarboxylic acid, 4-[[(6-methoxy-1,5-naphthyridin-4-yl)amino]carbonyl]-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)

RN 495414-91-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-(hydroxymethyl)-4-[[(6-methoxy-1,5-naphthyridin-4-yl)amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

```
L13
     ANSWER 4 OF 7 CAPLUS
                           COPYRIGHT 2005 ACS on STN
     2002:964146 CAPLUS
AN
DN
     138:39187
TТ
     Preparation of piperidinecarboxylates and related compounds as NMDA NR2B
     receptor antagonists for the treatment or prevention of migraine.
IN
     Allen, Christopher; Koblan, Ken S.; Sleeth, Timothy
     Merck & Co., Inc., USA
PA
                                              Commatricher
SO
     PCT Int. Appl., 185 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
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PΙ
     WO 2002100352
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                          A2
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     WO 2002100352
                         A3
                                20030327
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
             GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
             GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1399160
                                20040324
                                           EP 2002-744807
                         A2
                                                                   20020607
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004537526
                                20041216
                                            JP 2003-503178
                                                                   20020607
                          Т2
     US 2004204341
                          A1
                                20041014
                                            US 2003-479923
                                                                   20031205
PRAI US 2001-297672P
                          Ρ
                                20010612
     WO 2002-US21069
                          W
                                20020607
AB
     A method for treating or preventing migraines comprises administration of
     an NR2B receptor antagonist (no data). The invention also encompasses the
     combination of an NR2B antagonist with a cyclooxygenase-2 selective
     inhibitor, a calcitonin gene-related peptide receptor (CGRP) ligand, a
     leukotriene receptor antagonist, or a 5HT1B/1D agonist for the treatment
     or prevention of migraines. Thus, 4-hydroxybenzoic acid,
     1-hydroxybenzotriazole hydrate, benzyl 4-(aminomethyl)piperidine-1-
     carboxylate (preparation given), and Et3N in DMF were treated with
     1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and the mixture
     allowed to stir at room temperature for 18 h to give 4-[(4-
     hydroxybenzoylamino)methyl]piperidine-1-carboxylic acid benzyl ester.
IT
     455265-96-0P 455266-09-8P 478552-69-1P,
     4-(Quinolin-2-ylaminomethyl)piperidine-1-carboxylic acid benzyl ester
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of piperidinecarboxylates and related compds. as NR2B receptor
        antagonists for the treatment or prevention of migraine)
RN
     455265-96-0 CAPLUS
CN
     1-Piperidinecarboxylic acid, 4-[(4-pteridinylamino)methyl]-, phenylmethyl
     ester (9CI)
                 (CA INDEX NAME)
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RN 455266-09-8 CAPLUS

CN 4-Piperidinemethanamine, N-(4-amino-2-quinazolinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ S - CH_2 - CH_2 - Ph \\ \hline \\ N \\ NH_2 \end{array}$$

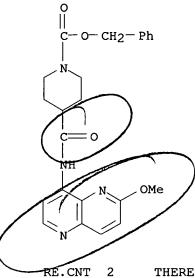
RN 478552-69-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(2-quinolinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

```
L13
    ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
     2002:927429 CAPLUS
AN
DN
     138:14011
TI
     Preparation of bicyclic nitrogen-containing heterocyclic derivatives for
     use as antibacterials
IN
     Dartois, Catherine Genevieve Yvette; Markwell, Roger Edward; Madler, Guy
     Marguerite Marie Gerard; Pearson, Neil David
PA
     Smithkline Beecham P.L.C., UK
SO
     PCT Int. Appl., 71 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 1
     PATENT NO.
                        KIND
                                DATE
                                           APPLICATION NO.
                                                                   DATE
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PΤ
     WO 2002096907
                         A1
                               20021205
                                          WO 2002-EP5709
                                                                 20020524
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                               20040303
                                          EP 2002-774022
                         A1
                                                                  20020524
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004534780
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                                20041118
                                          JP 2003-500086
                                                                   20020524
     US 2004198755
                         Α1
                                20041007
                                            US 2004-477900
                                                                   20040524
PRAI GB 2001-12836
                         Α
                                20010525
     WO 2002-EP5709
                         W
                                20020524
     MARPAT 138:14011
OS
AΒ
     Piperidine derivs. and pharmaceutically acceptable derivs. [I; wherein one
     of Z1, Z2, Z3, Z4, Z5 = N, one is CR2 (wherein R2 = H, OH, (C1-C6)alkoxy,
     etc.) and the remainder are CH, or one of Z1, Z2, Z3, Z4, Z5 = CR2 and the
     remainder are CH; R3 = H, carboxy, (C1-C6)alkoxycarbonyl, aminocarbonyl,
     cyano, tetrazolyl, etc.; R4 = U-V-R5, wherein U-\dot{V} = (CH2)2, CH2CH(OH),
     CH2CO, and R5 is a (substituted) bicyclic carbocyclic or heterocyclic ring
     system] were prepared For example, II was prepared by a multistep synthetic
     procedure. The prepared compds. are useful in the treatment of bacterial
     infections in mammals, particularly man. For example, compound II had MIC
     values ≤4 μg/mL against S. aureus Oxford.
ΙT
     477787-64-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of bicyclic nitrogen-containing heterocyclic derivs. for use as
        antibacterials)
     477787-64-7 CAPLUS
RN
```

1-Piperidinecarboxylic acid, 4-[[(6-methoxy-1,5-naphthyridin-4-yl)amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

CN



THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AN
     2002:676010 CAPLUS
     137:216875
DN
     Preparation of N-acyl-4-(heterocyclylaminomethyl)piperidines as NMDA/NR2B
ΤI
     antagonists
     Claiborne, Christopher F.; Butcher, John W.; Claremon, David A.; Libby,
IN
     Brian E.; Liverton, Nigel J.; Munson, Peter M.; Nguyen, Kevin T.;
     Phillips, Brian; Thompson, Wayne; McCauley, John A.
PA
     Merck & Co., Inc., USA
     PCT Int. Appl., 208 pp.
SO
     CODEN: PIXXD2
DT
     Patent
T.A
     English
FAN.CNT 1
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
     PATENT NO.
                                            ______
                                _____
PΙ
     WO 2002068409
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                                20020906
                                            WO 2002-US5226
                                                                    20020220
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2438895
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                                            CA 2002-2438895
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     US 2002165241
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                          A1
     EE 200300403
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                                20040114
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                20040309
                                            BR 2002-7526
                                                                    20020220
     BR 2002007526
                          Α
     JP 2004524314
                          T2
                                20040812
                                             JP 2002-567923
                                                                    20020220
                                            US 2003-470561
     US 2004209889
                          Α1
                                20041021
                                                                    20030729
     NO 2003003732
                          Α
                                20031022
                                            NO 2003-3732
                                                                    20030822
PRAI US 2001-271100P
                          Ρ
                                20010223
     WO 2002-US5226
                          W
                                20020220
     MARPAT 137:216875
     BQ1(X)ANHQ2 [Q1 = 5-7 membered N-containing nonarom. ring, azabicyclooctyl; Q2
AB
     = 5-6 membered (substituted) heteroaryl ring; A = alkylene; B =
     Ar(CH2)0-302C, Ar(CH2)0-3SO2, etc.; Ar = (substituted) aryl, heteroaryl; X
     = H, OH, F, alkyl, alkoxy, NH2, O], were prepared Thus,
     1-[(benzyloxy)carbonyl]-4-piperidinecarboxylic acid, 4-aminopyridine, EDC,
     and HOAt were kept 4 h in DMF to give the amide, which was reduced with
     BH3.THF to give benzyl 4-[(4-pyridylamino)methyl]-1-piperidinecarboxylate.
     Title compds. showed IC50's of <50 \mu M for inhibition of NR1A/2B NMDA
     receptor activation.
TT
     455265-29-9P 455265-96-0P 455266-09-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (claimed compound; preparation of
N-acyl-4-(heterocyclylaminomethyl)piperidine
        s as NMDA/NR2B antagonists)
RN
     455265-29-9 CAPLUS
     1-Piperidinecarboxylic acid, 4-[(4-quinolinylamino)methyl]-, phenylmethyl
CN
     ester (9CI) (CA INDEX NAME)
```

RN 455265-96-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-pteridinylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-09-8 CAPLUS

CN 4-Piperidinemethanamine, N-(4-amino-2-quinazolinyl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \parallel \\ S - CH_2 - CH_2 - Ph \\ \parallel \\ O \\ NH_2 \end{array}$$

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L13 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2001:372159 CAPLUS
- DN 134:366868
- TI Preparation of benzothiazolines as neuropeptide Y receptor antagonists
- IN Sato, Yoshiya; Itani, Hiromichi; Tabuchi, Seiichiro; Sakata, Yoshihiko; Ohashi, Hiroko
- PA Fujisawa Pharmaceutical Co., Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 88 pp. CODEN: JKXXAF
- DT Patent
- LA Japanese

FAN CNT 1

TAN.CNI I								
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
PI JP 2001139574	A2	20010522	JP 2000-296175	20000928				
PRAI AU 1999-3093	Α	19990928						

OS MARPAT 134:366868

AB The title compds. I [R1 = H, halo; W = S, O; A = (CH2)n, etc.; n = 1 - 6; Z = (un)substituted N-containing heterocyclic ring] are prepared 1-[(5-Chloro-2-oxobenzothiazolin-3-yl)acetyl]piperidine-4-carboxylic acid 4-benzoylanilide showed IC100 of 10-7 M in a neuropeptide Y5 receptor binding assay.

IT 340179-00-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzothiazolines as neuropeptide Y receptor antagonists)

RN 340179-00-2 CAPLUS

CN 4-Piperidinecarboxamide, 1-[(5-chloro-2-oxo-3(2H)-benzothiazolyl)acetyl]-N-6-quinolinyl- (9CI) (CA INDEX NAME)

=> => d his

(FILE 'HOME' ENTERED AT 15:31:29 ON 21 JAN 2005)

	FILE	'REGISTRY' ENTERED AT 15:31:40 ON 21 JAN 2005
L1		STRUCTURE UPLOADED
L2		0 S L1 SSS SAM
L3		STRUCTURE UPLOADED
L4		0 S L3 SSS SAM
L5		STRUCTURE UPLOADED
L6		0 S L5 SSS SAM
L7		SCREEN 1840
L8		SCREEN 2016 OR 2039 OR 2040 OR 2045 OR 2047
L9		STRUCTURE UPLOADED
L10		QUE L9 AND L7 NOT L8
L11		0 S L10 SSS SAM
L12		11 S L10 SSS FUL

FILE 'CAPLUS' ENTERED AT 15:45:10 ON 21 JAN 2005 L13 7 S L12

FILE 'CAOLD' ENTERED AT 15:45:42 ON 21 JAN 2005

=> s 112

L14 0 L12

=> log y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.43	206.46
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0 00	-5 11

STN INTERNATIONAL LOGOFF AT 15:45:53 ON 21 JAN 2005

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C:\Program Files\Stnexp\Queries\10079452
```

```
chain nodes :
                                    20
                                             22
                                                 23
                                                      27
                                                          29
                                                               30
                                                                   31
                                                                        32
                                                                            35
                                                                                36
                                                                                     37.
       8 9
              10
                  11
                       14
                           15
                                19
                                        21
    7
    46
        47
             48
                 167
ring nodes
                                                               57
                                                                    58
                                                                         59
                                                                             60
                                                                                  61
                            17 18
                                     51
                                         52 53 54
                                                      55
                                                          56
       2
              4
                 5
                     6
                       16
                                  69
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                                                                           81
                                                                               82 83
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                                       92
    84
             86
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         107
               108
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                                     112
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                                                                                  150
    151
         152
               153
                    154
                          155
                               156
chain bonds :
                                                    16-19
                                                           20-21
                                                                   20-22
                                                                           22-23
               7-9
                      9-10
                                   14-15
                                            14-18
    2-46
          7-8
                           10-11
                                           36-37
                                                          48-167
           27-30
                   30-31
                           31-32
                                   35-36
                                                  47-48
    27-29
ring bonds :
                    3 - 4
                          4-5
                               5-6
                                    16-17
                                            16-18
                                                     17-18
                                                            51-52
                                                                    51-56
                                                                            52-53
    1-2 1-6
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    53-54
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           54-55
                   55-56
                           55-57
                                   56-59
                                                                                  72-73
    63-64
            64 - 65
                   64-66
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    73-74
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                                                                  93-94
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    85-87
            86-89
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            96-97
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                        116-118
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                                            125-127
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    130-131
              130-135
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                                  132-133
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                        139-140
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    136-137
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                                            148-149
                                                      148-153
                        152-154
                                  153-156
                                            154-155
                                                      155-156
    151-152
              152-153
exact/norm bonds :
                                                7-9
                                      5-6
                                            7-8
    1-2 1-6 2-3
                    2-46
                           3-4 4-5
                                                       9-10 10-11
                                                                     14-15
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            16-18
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                                                          27-29
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    16-17
                   16-19
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                                                                          30-31
                                                                                  31 - 32
    35-36
            36-37
                   47 - 48
                           48-167
                                    55-57
                                            56-59
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                                                                   64-66
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                                           76-77 85-87
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    66~67
            67-68
                   73-75
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                                                                                  94-96
                                              109-110
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                   97-98
                           107-109 108-111
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    95-98
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    118-119
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119-120
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                     143-145 144-147
                                       145-146
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                                                                  153-156
    154-155
             155-156
normalized bonds :
                                                           61-62
                        53-54
                               54-55
                                                    60-65
   51-52 51-56 52-53
                                      55-56
                                             60-61
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           69-70
                 69-74
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                                                                         83-84
    64 - 65
    84-85
           85-86
                 90-91
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                                            93-94
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                                                           103-104
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    130-131
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    140-141
                     142-143
                              143-144
                                       148-149
                                                148-153
                                                         149-150
                                                                  150-151
    151-152
            152-153
isolated ring systems :
    containing 1 : 16 : 51 : 60 : 69 : 81 : 90 : 103 : 112 : 121 : 130 : 139 :
G1:0,N
G2:[*1],[*2],[*3],[*4],[*5]
G3:C,N
G4: [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13], [*14], [*15], [*16]
Match level :
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    1:Atom
                                           6:Atom
                                                   7:CLASS
                                                            8:CLASS
                                                                     9:CLASS
                                                            18:Atom
             11:Atom 14:CLASS 15:CLASS
    10:CLASS
                                          16:Atom
                                                   17:Atom
                                                                     19:Atom
                                23:Atom
             21:CLASS
                      22:CLASS
                                          27:CLASS
                                                  29:CLASS 30:CLASS
    20:CLASS
    31:CLASS
             32:Atom 35:CLASS
                                50:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom
    48:CLASS
    57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom
    65:Atom
            66:Atom 67:Atom 68:Atom
                                      69:Atom
                                               70:Atom
                                                        71:Atom
   73:Atom 74:Atom
                    75:Atom 76:Atom 77:Atom 81:Atom
                                                        82:Atom
   84:Atom 85:Atom 86:Atom 87:Atom
                                       88:Atom 89:Atom
                                                        90:Atom
            93:Atom 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
    92:Atom
   104:Atom 105:Atom 106:Atom 107:Atom
                                           108:Atom 109:Atom 110:Atom
                                 114:Atom
                                                     116:Atom
   111:Atom
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                       113:Atom
                                           115:Atom
                                                               117:Atom
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                                 156:Atom
                                           167:CLASS
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   Saturation
                          : Unsaturated
   Saturation
                          : Unsaturated
   23:
   Saturation
                          : Unsaturated
   32:
   Saturation
                          : Unsaturated
   37:
   Saturation
                          : Unsaturated
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Element Count :

Node 47: Limited C,C1-5

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1840

L1 SCREEN CREATED

=> screen 2016 OR 2039 OR 2040 OR 2045 OR 2047

L2 SCREEN CREATED

373635

chain nodes :
7 8 9 10 11 14 15 19 20 21 22 23 27 29 30 31 32 35 36 37 46 47
 48 167
ring nodes :
1 2 3 4 5 6 16 17 18 51 52 53 54 55 56 57 58 59 60 61 62 63
64 65 66 67 68 69 70 71 72 73 74 75 76 77 81 82 83 84 85 86 87
88 89 90 91 92 93 94 95 96 97 98 103 104 105 106 107 108 109 110
111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127
 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143
144 145 146 147 148 149 150 151 152 153 154 155 156
chain bonds :
2-46 7-8 7-9 9-10 10-11 14-15 14-18 16-19 20-21 20-22 22-23 27-29 27-30
 30-31 31-32 35-36 36-37 47-48 48-167

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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18 17-18 51-52 51-56 52-53 53-54
54-55 55-56 55-57 56-59 57-58 58-59 60-61 60-65 61-62 62-63 63-64 64-65
                                                                                   73-75 74-77
64-66 65-68 66-67 67-68 69-70 69-74 70-71 71-72 72-73 73-74
75-76 76-77 81-82 81-86 82-83 83-84 84-85 85-86 85-87 86-89 87-88 88-89
90-91 90-95 91-92 92-93 93-94 94-95 94-96 95-98 96-97 97-98 103-104
103-108 104-105 105-106 106-107 107-108 107-109 108-111 109-110 110-111
112-113 112-117 113-114 114-115 115-116 116-117 116-118 117-120 118-119
119-120 121-122 121-126 122-123 123-124 124-125 125-126 125-127 126-129
127-128 128-129 130-131 130-135 131-132 132-133 133-134 134-135 134-136
135-138 136-137 137-138 139-140 139-144 140-141 141-142 142-143 143-144
143-145 144-147 145-146 146-147 148-149 148-153 149-150 150-151 151-152
152-153 152-154 153-156 154-155 155-156
exact/norm bonds :
1-2 1-6 2-3 2-46 3-4 4-5 5-6 7-8 7-9 9-10 10-11 14-15 14-18 16-17
16-18 16-19 17-18 20-21 20-22 22-23 27-29 27-30 30-31 31-32 35-36 36-37
47-48 48-167 55-57 56-59 57-58 58-59 64-66 65-68 66-67 67-68 73-75 74-77
 75-76 76-77 85-87 86-89 87-88 88-89 94-96 95-98 96-97 97-98 107-109
108-111 109-110 110-111 116-118 117-120 118-119 119-120 125-127 126-129
127-128 128-129 134-136 135-138 136-137 137-138 143-145 144-147 145-146
146-147 152-154 153-156 154-155 155-156
normalized bonds :
                        53-54 54-55 55-56 60-61 60-65 61-62 62-63 63-64 64-65
51-52 51-56 52-53
69-70 69-74 70-71 71-72 72-73 73-74 81-82 81-86 82-83 83-84 84-85 85-86
90-91 90-95 91-92 92-93 93-94 94-95 103-104 103-108 104-105 105-106
106-107 107-108 112-113 112-117 113-114 114-115 115-116 116-117 121-122
121-126 122-123 123-124 124-125 125-126 130-131 130-135 131-132 132-133
133-134 134-135 139-140 139-144 140-141 141-142 142-143 143-144 148-149
148-153 149-150 150-151 151-152 152-153
isolated ring systems :
containing 1: 16: 51: 60: 69: 81: 90: 103: 112: 121: 130: 139: 148:
G1:0,N
G2: [*1], [*2], [*3], [*4], [*5]
G3:C,N
G4: [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13], [*14], [*15], [*16]
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS 23:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom
35:CLASS 36:CLASS 37:Atom 46:CLASS 47:CLASS 48:CLASS 50:CLASS 51:Atom
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      104:Atom
      105:Atom
      106:Atom
      107:Atom
      108:Atom
      109:Atom
      110:Atom
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      143:Atom

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152:Atom 153:Atom 154:Atom 155:Atom 156:Atom 167:CLASS
Generic attributes :
11:
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Saturation : Unsaturated

19:

Saturation : Unsaturated

23:

Saturation : Unsaturated

32:

Saturation : Unsaturated

37:

Saturation : Unsaturated

Element Count : Node 47: Limited

C,C1-5

L3 STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4 QUE L3 AND L1 NOT L2

=> d 14

L4 HAS NO ANSWERS

L1 SCR 1840

L2 SCR 2016 OR 2039 OR 2040 OR 2045 OR 2047

L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L4 $\,$ QUE $\,$ L3 AND L1 NOT L2 $\,$

=> s 14 sss sam

SAMPLE SEARCH INITIATED 15:59:37 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1354 TO ITERATE

73.9% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 24873 TO 29287

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L3 AND L1 NOT L2

=> s 14 sss ful

FULL SEARCH INITIATED 15:59:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 26225 TO ITERATE

100.0% PROCESSED 26225 ITERATIONS

8 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.02

L6 8 SEA SSS FUL L3 AND L1 NOT L2

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 161.76 161.97

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 15:59:53 ON 21 JAN 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 21 Jan 2005 VOL 142 ISS 5 FILE LAST UPDATED: 20 Jan 2005 (20050120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> => d his

(FILE 'HOME' ENTERED AT 15:58:41 ON 21 JAN 2005)

FILE 'REGISTRY' ENTERED AT 15:58:45 ON 21 JAN 2005

L1 SCREEN 1840

SCREEN 2016 OR 2039 OR 2040 OR 2045 OR 2047 L2

L3 STRUCTURE UPLOADED

L4OUE L3 AND L1 NOT L2

L5 0 S L4 SSS SAM L6

8 S L4 SSS FUL

FILE 'CAPLUS' ENTERED AT 15:59:53 ON 21 JAN 2005

=> s 16

L7 5 L6

=> d 17 1-5 bib, ab, hitstr

```
L7
     ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ΑN
     2003:221651 CAPLUS
DN
     138:238196
ΤI
     Preparation of biarylmethylaminopurines as potent cyclin/CDK inhibitors
     and antiproliferative agents.
IN
     Trova, Michael Peter
PA
     Albany Molecular Research, Inc., USA
SO
     PCT Int. Appl., 275 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                                DATE
     PATENT NO.
                         KIND
                                            APPLICATION NO.
                                                                    DATE
                                             -----
PΙ
     WO 2003022805
                          A2
                                20030320
                                            WO 2002-US28730
                                                                    20020909
     WO 2003022805
                          A3
                                20040122
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             CO, CR, CU, CZ, DÈ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                            US 2002-237530
     US 2003092909
                                20030515
                          Α1
                                                                    20020906
     US 6812232
                          B2
                                20041102
PRAI US 2001-318569P
                          Р
                                20010911
OS
     MARPAT 138:238196
AB
     Title compds. [I; R1 = H, alkyl, alkenyl, cycloalkyl, CH2CF3, CH2CH2CF3,
     CH(CF3)2; R2 = (substituted) Ph, naphthyl, pyridyl, pyrimidyl, thienyl,
     furyl, pyrrolyl, quinolinyl, isoquinolinyl, etc.; R3 = H, alkyl, alkenyl,
     (substituted) Ph, phenylalkyl, etc.; R4 = H, alkyl; R3R4 = atoms to form a
     5-8 membered ring; R5 = heterocycle; A = CH2, (CH2)2, (CH2)3, OCH2CH2,
     CHCH3; Y = H, OR1, NHR1, NHCOR3, NHSO2R3, etc.; Q = (CH2)n; n = 0-3; V =
     NH, O, S, CH2], were prepared Thus, title compound II was prepared and
     inhibited growth of BT-579, MCF7, and numerous other transformed cell
     lines with GI50 < 0.01 \mu M.
IT
     441055-93-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of biarylmethylaminopurines as potent cyclin/CDK inhibitors and
        antiproliferative agents)
RN
     441055-93-2 CAPLUS
CN
     1-Piperidinecarboxylic acid, 4-[[[6-[([1,1'-biphenyl]-4-ylmethyl)amino]-9-
     (1-methylethyl)-9H-purin-2-yl]amino]methyl]-, phenylmethyl ester (9CI)
```

(CA INDEX NAME)

$$\begin{array}{c} & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

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L7
     ANSWER 2 OF 5 CAPLUS
                            COPYRIGHT 2005 ACS on STN
     2003:221467 CAPLUS
AN
DN
     138:255243
ΤI
     Preparation of biarylmethylaminopurines as potent cyclin/CDK inhibitors
     and antiproliferative agents
IN
     Trova, Michael Peter
PA
     Albany Molecular Research, Inc., USA
SO
     PCT Int. Appl., 266 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
                                DATE'
     PATENT NO.
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                                             APPLICATION NO.
                                                                    DATE
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             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                            US 2001-950543
     US 2003087906
                                20030508
                                                                    20010911
                          Α1
     US 6667311
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     US 2004077666
                          A1
                                20040422
                                            US 2003-680832
                                                                    20031007
PRAI US 2001-950543
                          Α
                                20010911
OS
     MARPAT 138:255243
AB
     The compds. I of the present invention are 2,6,9-trisubstituted purine
     derivs. which are inhibitors of cyclin/CDK complexes. Title compds. I [R1
     = H, alkyl, alkenyl, cycloalkyl, CH2CF3, CH2CH2CF3, CH(CF3)2; R2 =
     (substituted) Ph, naphthyl, pyridyl, pyrimidyl, thienyl, furyl, pyrrolyl,
     quinolinyl, isoquinolinyl, etc.; R3 = H, alkyl, alkenyl, (substituted) Ph,
     phenylalkyl, etc.; R4 = H, alkyl; R3R4 = form a 5-8 membered ring; R5 =
     heterocycle; A = CH2, (CH2)2, (CH2)3, OCH2CH2, CHCH3; Y = H, OR1, NHR1,
     NHCOR3, NHSO2R3, etc.; Q = (CH2)n; n = 0-3; V = NH, O, S, CH2], were
     prepared Thus, title compound II was prepared and inhibited growth of BT-579,
     MCF7, and numerous other transformed cell lines with GI50 < 0.01 \mu M.
     The compds. of the current invention also are potent inhibitors of human
     cellular proliferation. As such, the compds. of the present invention
     constitute pharmaceutical compns. with a pharmaceutically acceptable
     carrier. Such compds. are useful in treating a disorder mediated by
     elevated levels of cell proliferation in a mammal compared to a healthy
     mammal by administering to such mammal an effective amount of the compound
IT
     441055-93-2P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of biarylmethylaminopurines as potent cyclin/CDK inhibitors and
        antiproliferative agents)
RN
     441055-93-2 CAPLUS
CN
     1-Piperidinecarboxylic acid, 4-[[[6-[([1,1'-biphenyl]-4-ylmethyl)amino]-9-
     (1-methylethyl)-9H-purin-2-yl]amino]methyl]-, phenylmethyl ester (9CI)
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(CA INDEX NAME)

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1.7
     ANSWER 3 OF 5 CAPLUS
                           COPYRIGHT 2005 ACS on STN
     2002:964146 CAPLUS
AN
DN
     138:39187
ΤI
     Preparation of piperidinecarboxylates and related compounds as NMDA NR2B
     receptor antagonists for the treatment or prevention of migraine.
     Allen, Christopher; Koblan, Ken S.; Sleeth, Timothy
IN
PA
     Merck & Co., Inc., USA
     PCT Int. Appl., 185 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                                            APPLICATION NO.
                         KIND
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                         A2
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             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
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                         T2
                                20041216
                                           JP 2003-503178
                                                                   20020607
                                                                   20031205 NO
     US 2004204341
                                20041014
                                            US 2003-479923
                          A1
PRAI US 2001-297672P
                                20010612
                          Ρ
     WO 2002-US21069
                          W
                                20020607
     A method for treating or preventing migraines comprises administration of
AB
     an NR2B receptor antagonist (no data). The invention also encompasses the
     combination of an NR2B antagonist with a cyclooxygenase-2 selective
     inhibitor, a calcitonin gene-related peptide receptor (CGRP) ligand, a
     leukotriene receptor antagonist, or a 5HT1B/1D agonist for the treatment
     or prevention of migraines. Thus, 4-hydroxybenzoic acid,
     1-hydroxybenzotriazole hydrate, benzyl 4-(aminomethyl)piperidine-1-
     carboxylate (preparation given), and Et3N in DMF were treated with
     1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and the mixture
     allowed to stir at room temperature for 18 h to give 4-[(4-
     hydroxybenzoylamino) methyl] piperidine-1-carboxylic acid benzyl ester.
     455265-23-3P 455265-87-9P 455265-92-6P
IT
     455266-10-1P 455266-16-7P 455266-18-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of piperidinecarboxylates and related compds. as NR2B receptor
        antagonists for the treatment or prevention of migraine)
RN
     455265-23-3 CAPLUS
CN
     1-Piperidinecarboxylic acid, 4-[(1H-purin-6-ylamino)methyl]-, phenylmethyl
     ester (9CI) (CA INDEX NAME)
```

RN 455265-87-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(1H-pyrrolo[2,3-d]pyrimidin-4-ylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-92-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(1H-imidazo[4,5-c]pyridin-4-ylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-10-1 CAPLUS
CN 4-Piperidinemethanamine, N-(9-methyl-9H-purin-6-yl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$O = S - CH_2 - CH_2 - Ph$$

$$CH_2$$

$$NH$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

RN 455266-16-7 CAPLUS
CN 4-Piperidinemethanamine, N-1H-imidazo[4,5-b]pyridin-5-yl-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455266-18-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-1H-purin-2-yl-(9CI) (CA INDEX NAME)

IT 455265-50-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of piperidinecarboxylates and related compds. as NR2B receptor antagonists for the treatment or prevention of migraine)

RN 455265-50-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-amino-1H-purin-6-yl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

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1.7
     ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN
     2002:676010 CAPLUS
DN
     137:216875
ΤI
     Preparation of N-acyl-4-(heterocyclylaminomethyl)piperidines as NMDA/NR2B
     antagonists
     Claiborne, Christopher F.; Butcher, John W.; Claremon, David A.; Libby,
IN
     Brian E.; Liverton, Nigel J.; Munson, Peter M.; Nguyen, Kevin T.;
     Phillips, Brian; Thompson, Wayne; McCauley, John A.
PA
     Merck & Co., Inc., USA
SO
     PCT Int. Appl., 208 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                           APPLICATION NO.
                                                                   DATE
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             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
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     CA 2438895
                                20020906
                                           CA 2002-2438895
                          AΑ
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     US 2002165241
                                            US 2002-<u>79452</u>
                          A1
                                20021107
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                                                                   20020220
     EP 1379520
                          A1
                                20040114
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     BR 2002007526
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                         A
                                20040309
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     JP 2004524314
                          T2
                                                                   20020220
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     US 2004209889
                                            US 2003-470561
                          A1
                                                                   20030729
                                20041021
     NO 2003003732
                                            NO 2003-3732
                         Α
                                20031022
                                                                   20030822
PRAI US 2001-271100P
                          Р
                                20010223
                          W
     WO 2002-US5226
                                20020220
     MARPAT 137:216875
OS
AB
     BQ1(X)ANHQ2 [Q1 = 5-7 membered N-containing nonarom. ring, azabicyclooctyl; Q2
     = 5-6 membered (substituted) heteroaryl ring; A = alkylene; B =
     Ar(CH2)0-302C, Ar(CH2)0-3S02, etc.; Ar = (substituted) aryl, heteroaryl; X
     = H, OH, F, alkyl, alkoxy, NH2, O], were prepared Thus,
     1-[(benzyloxy)carbonyl]-4-piperidinecarboxylic acid, 4-aminopyridine, EDC,
     and HOAt were kept 4 h in DMF to give the amide, which was reduced with
     BH3.THF to give benzyl 4-[(4-pyridylamino)methyl]-1-piperidinecarboxylate.
     Title compds. showed IC50's of <50 \muM for inhibition of NR1A/2B NMDA
     receptor activation.
TΤ
     455265-23-3P 455265-50-6P 455265-87-9P
     455265-92-6P 455266-10-1P 455266-16-7P
     455266-18-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (claimed compound; preparation of
N-acyl-4-(heterocyclylaminomethyl)piperidine
        s as NMDA/NR2B antagonists)
RN
     455265-23-3 CAPLUS
     1-Piperidinecarboxylic acid, 4-[(1H-purin-6-ylamino)methyl]-, phenylmethyl
CN
     ester (9CI) (CA INDEX NAME)
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RN 455265-50-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[(2-amino-1H-purin-6-yl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-87-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(1H-pyrrolo[2,3-d]pyrimidin-4-ylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455265-92-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(1H-imidazo[4,5-c]pyridin-4-ylamino)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 455266-10-1 CAPLUS

CN 4-Piperidinemethanamine, N-(9-methyl-9H-purin-6-yl)-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$O = S - CH_2 - CH_2 - Ph$$

$$CH_2$$

$$NH$$

$$N$$

$$N$$

$$Me$$

RN 455266-16-7 CAPLUS

CN 4-Piperidinemethanamine, N-1H-imidazo[4,5-b]pyridin-5-yl-1-[(2-phenylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 455266-18-9 CAPLUS

CN 4-Piperidinemethanamine, 1-[(2-phenylethyl)sulfonyl]-N-1H-purin-2-yl-(9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L7
     ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
     2002:522682 CAPLUS
ΑN
DN
     137:78811
ΤI
     Preparation of 2,6,9-trisubstituted purine derivatives for therapeutic use
     as potent antiproliferative agents
IN
     Trova, Michael Peter
PA
     U.S. Pat. Appl. Publ., 150 pp., Cont.-in-part of U.S. Ser. No. 493,790.
SO
     CODEN: USXXCO
DT
     Patent
LA
     English
FAN.CNT 2
     PATENT NO.
                                            APPLICATION NO.
                         KIND
                                DATE
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             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
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     US 2004063727
                          A1
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                          P
PRAI US 1999-124829P
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     US 2000-493790
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     US 2001-950549
                          Α
                                20010911
os
     MARPAT 137:78811
AB
     2,6,9-Trisubstituted purine derivs., such as I [R = -VCH(R3)(CH2)nCH(R4)Y;
     R1 = H, alkyl, alkenyl, cycloalkyl, etc.; R2 = aryl, heteroaryl; R3 = H,
     alkyl, alkenyl, phenylalkyl, etc.; R4 = H, alkyl; R3(CH2)nR4 = 5-8
     membered carbocyclic or heterocyclic ring; A = CH2, CH2CH2, CH2CH2CH2,
     OCH2CH2, CH(Me), etc.; V = NH, O, S, CH2; X = N, CH; Y = H, alkyloxy,
     amino, acylamino, sulfonylamino, etc.; n = 0-3] which are inhibitors of
     cyclin/cdk complexes, were prepared for pharmaceutical use as antitumor
     agents. Thus, substituted purine II was prepared via a series of synthetic
     steps which included 6-amination of 2,6-dichloropurine with
     4-I-C6H4CH2NH2.HCl, 9-N-alkylation of the resulting purine with Me2CHI,
     2-amination of the resulting purine with trans-1,4-cyclohexanediamine and,
     finally, aromatic coupling of the 4-iodobenzyl moiety with 3-thiophene
     boronic acid. The prepared purines were assayed for cyclin/cdk inhibition
     and for growth inhibition of HeLa as well as a number of other cancer cell
     lines.
IT
     441055-93-2P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of 2,6,9-trisubstituted purine derivs. for therapeutic use as
       potent antiproliferative agents)
RN
     441055-93-2 CAPLUS
CN
     1-Piperidinecarboxylic acid, 4-[[[6-[([1,1'-biphenyl]-4-ylmethyl)amino]-9-
```

(1-methylethyl)-9H-purin-2-yl]amino]methyl]-, phenylmethyl ester (9CI)

(CA INDEX NAME)